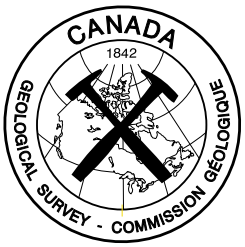

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Open File 4941

The measurement of the modal mineralogy of rocks from SEM imagery: the use of Multispec © and ImageJ freeware

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Note: This report has been formatted for double-sided printing

THE MEASUREMENT OF THE MODAL MINERALOGY OF ROCKS FROM SEM IMAGERY: THE USE OF MULTISPEC © AND IMAGEJ FREEWARE

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1. IMAGE ANALYSIS OF X-RAY MAPS

1. Introduction

The modal mineralogical analysis of rocks by image analysis of backscattered electron (BSE) images or X-Ray micrographs is hampered by the high proportion of pixels which contain signatures from more than one mineral at grain boundaries. In solid rock samples, these edge effect pixels cannot be compensated by methods such as dilation-erosion used by the conventional greyscale segmentation of grain mounts. Compensation of these edge effect pixels can be achieved by graphical or statistical methods using freeware computer programs.

ImageJ (Rasband, 1997) is a conventional image analysis application which allows modal mineralogical analysis to be accomplished by greyscale segmentation. In this method, a specific mineral is given a unique greyscale range by combining two or more X-Ray maps, with or without a BSE image, and then the number of pixels within this greyscale range are counted and converted to an area % by normalizing the pixel count to the total number of pixels in the image area. The upper and lower threshold values of the greyscale range are chosen so as to include about half the edge effect pixels associated with the mineral of interest. The threshold values are determined graphically from examination of histograms of greyscale values or profiles of greyscale values across mineral grain boundaries.

An alternative to greyscale segmentation is to statistically analyse the matrix of greyscale values which formed by a series of overlaid X-Ray maps to determine clusters with similar statistical distributions. *Multispec*© (Biehl and Landgrebe, 2002) is a multispectral image data analysis software application whose creation was inspired by the need for a readily available, easy to use, system that utilized new but complex analysis tools for multispectral data from earth observational satellites. The greyscale values of a series of X-Ray maps for different elements are ideal candidates for such an analysis because each mineral has its own distinctive chemical signature.

The great majority of greyscale segmentation techniques reported in the literature utilizes image analysis software that is part of the SEM operating system and available only to licensed users (e.g. Petruk, 1989; Lastra et al., 1998). The advantage of using *ImageJ* is that the modal mineralogical analysis using the greyscale segmentation technique can be carried out independently of the SEM system, thereby freeing the operator and the system for other tasks.

The use of multispectral data analysis software to carry out modal mineralogical analysis is relatively new (Hicks et al., 2002), but commercial multispectral software is not within the reach of many users. The ready availability of *Multispec*© makes this method available to all.

1.1. Greyscale rendition of X-Ray maps.

X-Ray maps produced by SEM imaging are most commonly rendered as 512 x 512 pixel greyscale images, though 1024 x 1024 pixel images are produced by some systems. The scaling of the greyscale value of a pixel to the X-Ray count for that beam position is usually manually carried out

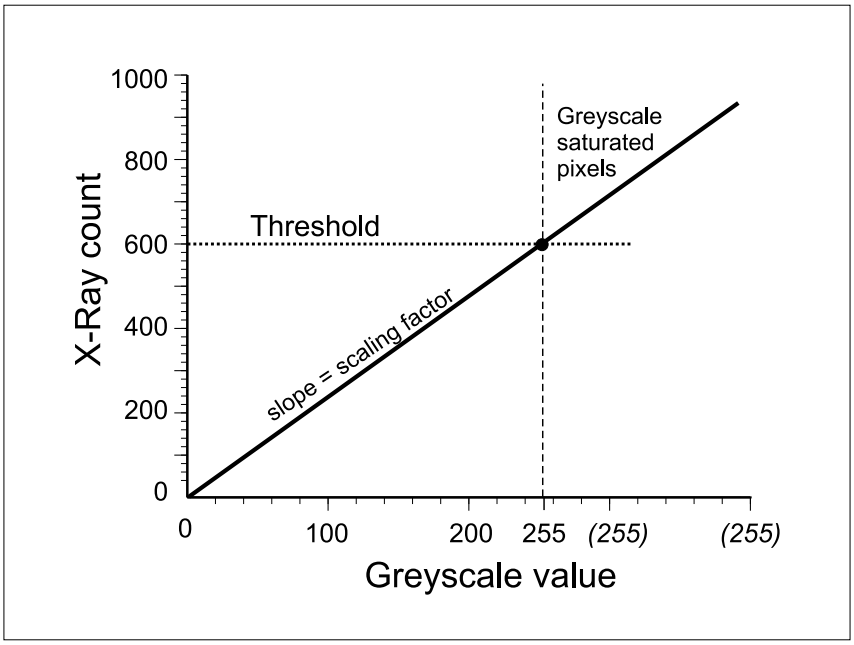


Fig. 1.1 Diagrammatic representation of the rendition of the X-Ray count at a point on the sample as a greyscale pixel of an X-Ray map. The X-Ray count is rendered as a greyscale value by the linear relationship given by the slope of the thick solid line. The slope of this line is determined by the operator's choice of a threshold value (in the diagram it is shown as 600 X-Ray counts), because the line passes through the origin of the diagram and the point at which the threshold value would have a greyscale value of 255. All pixels with an X-Ray count greater than the threshold value are rendered with the maximum greyscale value of 255 (white), and are referred to in this manual as greyscale saturated pixels. For X-Ray maps intended to be used for modal mineralogical measurement, the threshold should be set at the maximum X-Ray count for the element of interest.

by the SEM operator (see Fig. 1.1). For each X-Ray map, the operator decides on a threshold X-Ray count. Beam positions with an X-Ray count above this threshold value are all rendered white (greyscale value of 255) on the image. The greyscale value of the remaining beam positions are rendered by a linear scaling of the X-Ray between 0 and the threshold value to the greyscale range of 0-255.

The most common use of X-Ray maps is to determine or illustrate the spatial distribution of a selected element in a sample. For this purpose it is desirable that areas containing the highest concentration of the element of interest be visually distinct from the remainder of the image area. To achieve this visual effect the operator usually chooses a threshold X-Ray count that is less than the maximum X-Ray count for an element of interest, so that all areas with high concentrations of that element of interest are shaded white on the X-Ray map (greyscale value of 255) and contrast with the darker shades of the areas of the image containing lesser concentrations of that element. In this manual, such an image is termed "greyscale saturated".

However, for the purposes of modal mineralogical measurement, whether by greyscale segmentation or by statistical cluster analysis, it is preferable that the entire range of X-Ray counts be preserved in their greyscale rendition to enable the detection of small differences in the relative concentrations of the element when that element is a major constituent of a mineral. Therefore, for X-Ray maps required for modal mineralogical measurement, the threshold should be set at the maximum X-Ray count for the element, so that all pixels of the X-Ray map are scaled in linear proportion to their X-Ray count. This usually has the effect of produc-

ing an X-Ray map that is much darker than X-Ray maps that are produced for illustrating element distributions.

Another factor that affects X-Ray maps used for modal mineralogical analysis, more so than than it does for those images used just for illustrating element distribution, is instrument drift during collection of the X-Ray data. This may causes a change in the relationship between element concentration and X-Ray count from the top to the bottom of the X-Ray map. A method for identifying and correcting instrument drift is described on page 29.

1.2 Edge effect pixels of X-Ray maps.

Edge effects arise primarily both because the source of back-scattered electrons and X-Ray emission is a volume of sample that extends both below the surface and laterally away from the area of impingement of the electron beam (Fig. 1). At grain boundaries, the volume of electron excitement transects the different grains, and so the backscatter or secondary X-Ray response contains

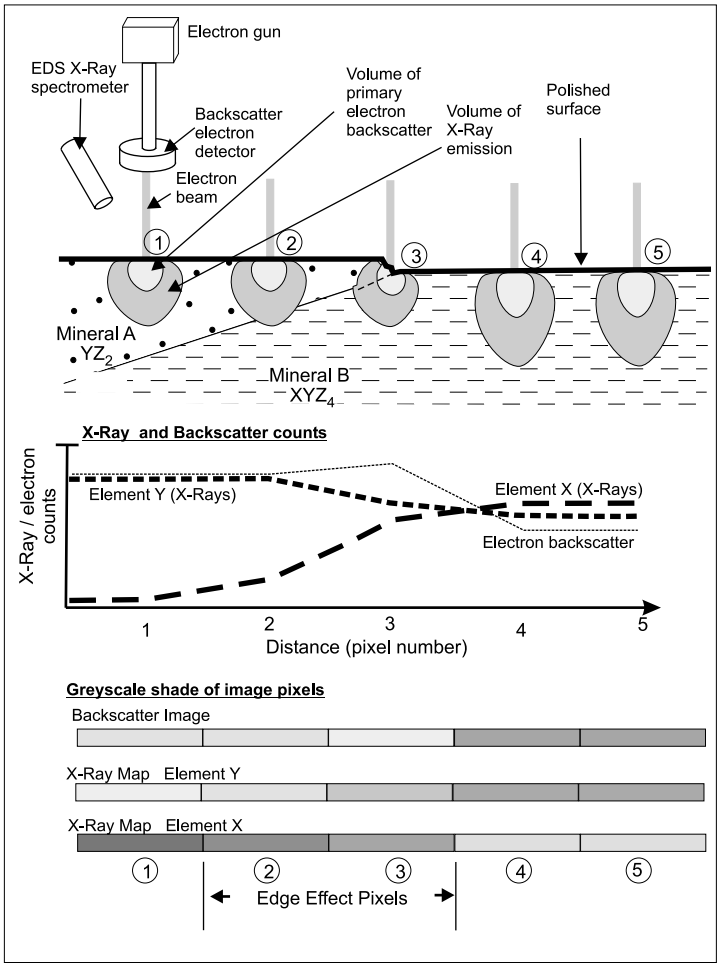


Fig. 1.2. Schematic representation of the scanning electron microscope generation and measurement of primary backscattered electrons and X-Ray emission from a polished rock , illustrating the effects of some of the variables involved and the generation of edge effect pixels. Element Y has a much higher atomic number than Element X which results in less depth penetration by incident electrons in Mineral A (chemical formula YZ_2) than mineral B (chemical formula XYZ_4) . Surface irregularity at the contact between MIneral A and Mineral B causes a higher proportion of electron backscatter. Note that X-Ray edge effect pixels are asymmetrically distributed about the mineral grain contact at the surface of the polished surface, extending further into the mineral whose contact forms an an acute angle with the polished surface, and that the BSE image more precisely maps the contact than the X-Ray image.

signatures of both minerals. Pixels representing these hybrid responses are termed "edge effect pixels (see Fig. 33). The depth of penetration of the electron beam depends on the chemical composition of the mineral. Elements with higher atomic numbers attenuate electron penetration more rapidly than elements with lower atomic numbers (e.g. Krinsley et al., 1998). The depth of penetration is also affected by surface irregularity of the sample, which causes differences in the angle of incidence of the electron beam with the sample surface, and consequently variation to the proportion of the electron that penetrates into the sample. Surface irregularity of polished rock samples is particularly common at grain boundaries, where contrasting hardness and mechanical strength of different minerals results in differential abrasion during the polishing process and a difference surface elevation between different grains. Plucking, especially of wedge-shaped contacts of weaker minerals, adds to grain boundary surface irregularity (Fig. 1.2).

The magnitude of the electron backscatter and X-Ray emission from the two different minerals is not a direct function of the distance of the grain boundary at the polished surface, but also depends on the angle of the grain contact with the polished surface. The response from the mineral forming the obtuse angle extends further from the grain contact than the mineral forming the acute angle (Fig. 1.2). The smaller the acute angle, and the greater transparency to electron penetration of the mineral that forms the acute angle, the further from the grain boundary edge effects will occur. The corridor of edge effect is therefore most commonly asymmetrically disposed with respect to the optical grain contact at the polished surface.

The complexity of the relationship of edge effect pixels to the minerals grains that contribute to their signature is further increased by the relative electron transparency of the minerals involved. Because the volume excited by electron bombardment is larger in minerals with average low atomic number than minerals with average higher atomic number, X-Ray signatures of the former will tend to extend further from the grain boundary than signatures of the latter. The multitude of factors that contribute to edge effects means that there is not a simple method for apportioning edge-effect pixels to one mineral or the other, either numerically in terms of greyscale pixel values, such as the average of the greyscale ranges of both minerals, or graphically, such as equidistance between pixels that mark the boundaries of "pure" mineral. This article describes the various methods by which edge effect pixels are assigned to mineral classes when using the protocols for greyscale segmentation with *ImageJ* and statistical classification using *Multispec*©.

2. MODAL MINERALOGICAL ANALYSIS USING *IMAGEJ*

2. Introduction

ImageJ works by allowing mathematical manipulation and measurements of a single, composite (single layer derived by amalgamating several single layers) or multiple layers (a stack) of grey scale bitmaps. The capabilities of *ImageJ* that are used here, is its capability to measure the thresholded area of a composite X-Ray image that has been segmented to reflect a single mineral species. The boundary of the species is manually determined from consideration of histograms and profiles across grain boundaries. To eliminate the edge effect problem that the same pixel may be selected for different minerals (or, alternatively, not selected for any mineral), the technique used here adopts the same philosophy that is used to calculate normative mineralogy of a rock from a whole rock chemical analysis. That is by selecting a mineral in order of a pre-determined selection hierarchy, and successively subtracting these minerals from the whole. To do this with X-Ray maps, a knowledge of the minerals of the rock sample is therefore a prerequisite to decide the most appropriate hierarchy.

General procedure

The general procedure for a complete modal mineralogical analysis of the sample by greyscale segmentation using *ImageJ* involves:

1) gaining familiarity with the range of minerals in the sample;
2) deciding which SEM images or combinations thereof gives a good greyscale separation for a specific mineral;
3) thresholding the image to select only the mineral of interest;
4) measuring the thresholded areas of the image;
5) eliminating measured areas from the image so that they will not be incorporated into subsequent measurements.
6) Production of a table of results and a mineral distribution map.

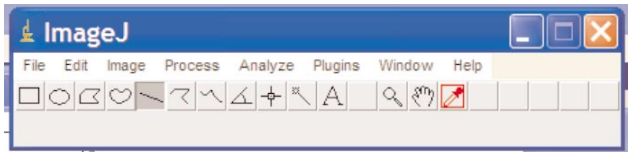


Fig.2 The main menu bar of ImageJ. In this manual, the first-listed command of command chains written in italics refers to a selection from this menu.

2.1. Gaining familiarity with the range of minerals in the sample.

Familiarity with the range of different minerals in the sample is best gained by prior petrography. Within ImageJ there are several routines which help with mineral diagnosis:

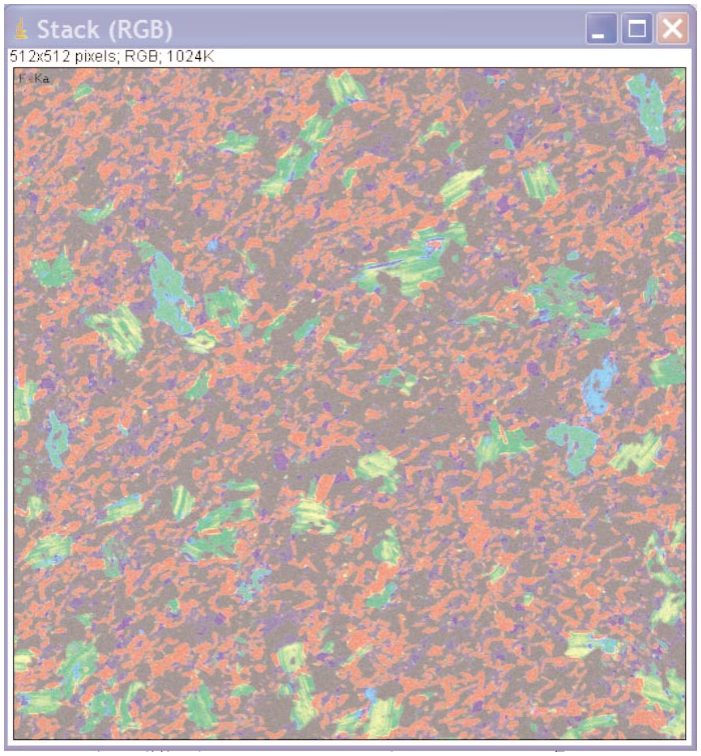


Fig. 3 RGB projection of a three-layer stack of X-Ray maps using the *Image->Color->Convert Stack to RGB* command. The X-Ray maps were opened in the order of potassium (red), iron (green) and calcium (blue). Muscovite shows as red, biotite as yellow, chlorite as yellowish green, ilenite as bluish green, titanite as light blue, feldspar and apatite as dark blue, epidote as turquoise, quartz as black.

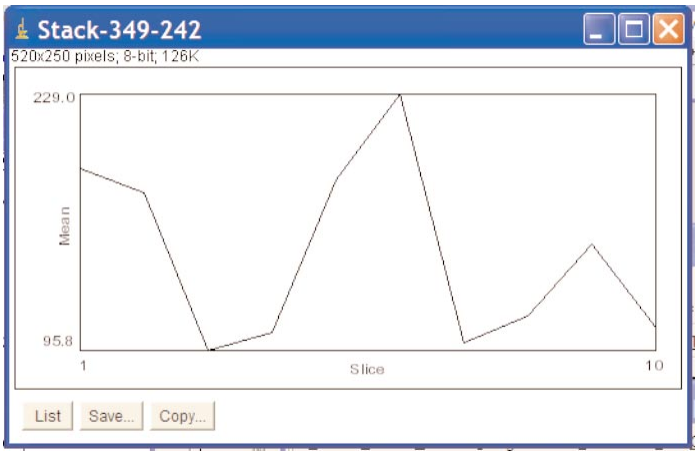


Fig.4 Vertical profile through a stack of ten elements (sorted alphabetically from Al on the left to Ti on the right) produced by the *Image->Stacks-Plot Z-axis* profile on a selection of four pixels of a feldspar grain.

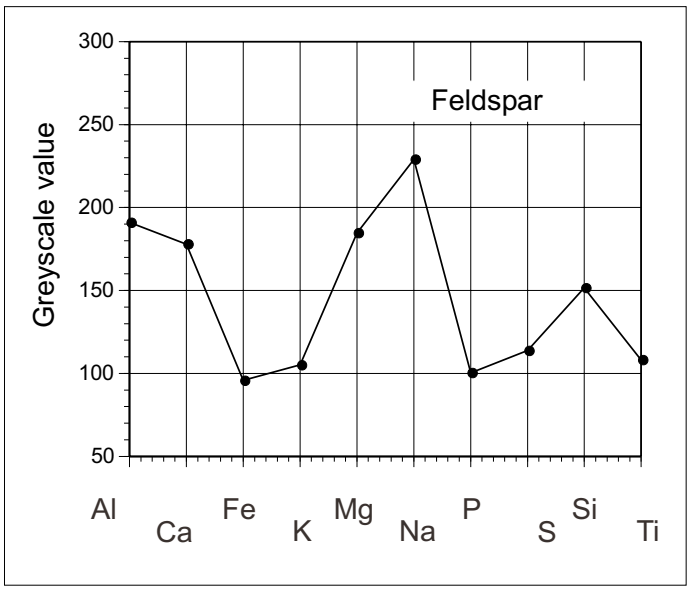


Fig. 5. The profile of Fig. 4 replotted in graphing software by copying and pasting the numerical data, which is obtained by clicking the "List" button shown in Fig. 4 .and adding the labeling (by using a template to save time).

2.1.1. Three element colour maps.

Inspection of a coloured composite image of three X-Ray maps of different elements, in which the different elements are assigned to red, blue and green respectively, is a very useful tool for identifying the distribution of the different mineral species (Fig. 2). This is done by:

i). Opening the X-Ray maps in **.tif* format in the order desired for red, blue and green via successive use of the *File->Open* command.

ii). Use the *Image->Stacks->Convert Images to Stack* and then the *Image->Color->Convert Stack to RGB* commands.

It should be noted that before creating a map with a different set of elements, all image windows must be closed. It should be further noted that a three element colour projection of greyscale X-Ray maps is much more readily carried out using *Multispec*© (see page 18).

2.1.2. Multi-element profile of a small group of pixels.

Another useful tool in *ImageJ* is the routine for drawing a vertical profile through a stack, which can be used to construct a multi-element spectrum of a single pixel or the average greyscale value of a part of a selected mineral (Fig.4). This spectrum is very useful for identifying all the chemical constituents of a mineral and hence an identification of an unknown mineral which might have shown up as being distinctive on a RGB stack. The multi-element stack is most conveniently created by:

iii) Create a computer folder or sub-directory holding only the X-Ray images in *.tif format. The images should be renamed so that the different maps, when sorted in ascending order, will be in the order required for the profile.

iv.) Use the *File->Import-> Image Sequence* command on a computer folder or sub-directory that contains only the X-Ray maps. Note that this command works even if windows of a three element stack and its RGB projection are also open, unlike creating a stack from the *Image->Convert Images to Stack* command.

v) Scroll the stack, by using the slider at the bottom of the stack image, to an X-Ray Map in which the mineral of interest can be distinguished. Select one or more pixels of the mineral of interest in the mult-element stack window by using the rectangular select tool, and using the *Image->Stacks->Plot Z-axis Profile* command. A plot similar to Fig. 4 is produced.

The graphics for profiles, histograms and plots produced by *ImageJ* are rudimentary (e.g. Fig. 4). A better quality of graphics may be produced by plotting the raw data with an independant graphics software application, as in the example of Fig. 5. The data for each graphics window can be listed as

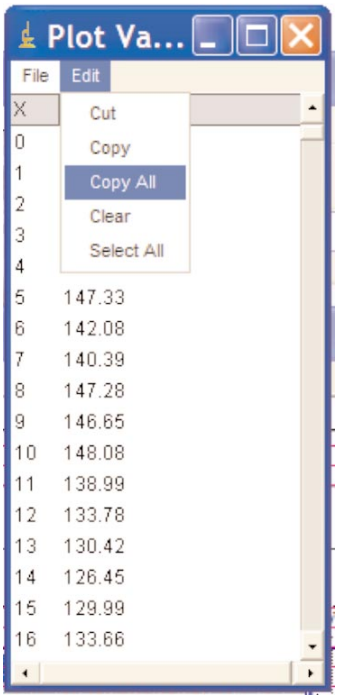


Fig. 6. Example of a data text window obtained by clicking on the "List" button of a graphics window. The data is copied to the clipboard by using the "Edit-Copy All" command as illustrated, and then may be pasted into the data sheets of a graphics software application.

text columns and rows by clicking on the "List"button (as in Fig. 4) to produce a text window as in Fig. 6, then using the "Edit->Copy All" command of this text window to copy the data on to the clipboard.

The greyscale values for most X-Ray maps are not calibrated against content of the element in the mineral. Usually individual maps are calibrated such that the maximum content of the element in the image area has a greyscale approaching 255 (white). Thus the relative greyscale values of the different elements do not indicate relative proportions of the element is in the mineral. In interpreting a profile such as the one for plagioclase feldspar shown in Fig. 4 and Fig. 5, the different greyscale relationships to element contents for the different X-Ray maps must be borne in mind. Some images, especially when the main intent of the X-Ray map was to show the distribution of a specific mineral, may be oversaturated so that all contents in excess of a certain value have a greyscale value of 255. This is the case for Mg in Fig 5, so its high greyscale value in relation to Al, Ca, Na and Si (the main feldspar-forming elements in the X-Ray stack) should be ignored for the set of X-Ray maps illustrated here.

Order of measurement	Mineral identified and measured	X-Ray maps used	Significance of pixels with highest greyscale values
1	Monazite	P plus Inverted Ca.	Minerals containing P but not Ca
2	Apatite	P plus *Cumulative 1	Contains all remaining Phosphorous
3	Pyrrhotite	S plus *Cumulative 2	Only sulphide in sample.
4	Rutile	3xTi plus Inv Fe plus Inv Ca plus *Cumulative 3	Minerals containing high Ti but low Fe and/or low Ca
5	Titanite	Ti plus Ca plus *Cumulative 4	Remaining minerals containing Ti and Ca
6	Ilmenite	Ti plus *Cumulative 5	Remaining minerals containing major Ti
7	Quartz	Si plus *Cumulative 6	Remaining minerals with the highest Si.
	(Total remaining Iron minerals - *TRFe)	Fe plus *Cumulative 7	Remaining minerals with high Fe
8	Epidote	Ca plus Inverted *TRFe	Minerals with high Ca and high Fe
9	Biotite	K plus *Inverted *TRFe plus *Cumulative 8	Minerals containing high Fe and high K
10	Chlorite	Al plus *Inverted *TRFe plus *Cumulative 9	Remaining minerals containing high Fe and Al (does not include carbonates or oxides)
11	Muscovite	K plus Inverted Na plus Cumulative 10	Remaining minerals with high K (Inverted Na image helps to give a better bimodal
12	Calcite	Ca plus Cumulative 11	Remaining minerals containing the highest Ca
13	Feldspar	Na plus Cumulative 12	Remaining minerals containing Na
14	Unclassified	Inverted Cumulative 13	Pixels not classified

Table 1. Example of the order in which minerals are segmented and measured and the X-Ray images used. r the greyscale segmentation of minerals using ten X-Ray maps for Al, Ca, Fe, K, Mg, Na, P, S, Si, and Ti.
Notes:
* signifies a binary file in which the area of interest is black.
"Cumulative" is a summation of areas of all previously measured minerals.
"Inverted" is a reversal of the greyscale (i.e. 255 minus original greyscale value)

2.2. Deciding which SEM images or combinations thereof gives a good greyscale separation for a specific mineral.

The aim of image selection for greyscale segmentation is to choose an X-Ray map, or combination of maps, which gives the mineral of interest a unique greyscale range compared to other minerals in the image area. Most conveniently, this greyscale range should be at the high end of the greyscale range of the image (i.e. light shades or high abundances of selected elements) and all other pixels are at the low end. A light shade for the mineral of interest is obtained by making a composite X-Ray map made by the greyscale addition of X-Ray maps for the elements that the mineral of interest contains. In some cases, one X-Ray map may suffice.

The order in which mineral areas are measured affects the precise result obtained, because of ambiguities in the methods of compensating for the edge-effect problem. The challenge is to determine a hierarchy of minerals such that the segmentation of one does not unduly affect the segmentation and measurement of another. A convenient rule of thumb is to: 1) first segment minerals whose elimination will entirely remove a chemical component from the whole; and then 2) successively choose minerals with a unique combination of the remaining elements that will progressively eliminate an element. An hierarchy of minerals for the sample considered here is listed in Table 1.

In some cases, it is advantageous to use a mask to black-out the entire image area except those of certain minerals. For example, in the case considered here, its is desirable to isolate epidote, biotite and chlorite from the remaining minerals to be classified, so that they can be independently segmented based on their calcium and potassium contents. The image in Fig. 7a was created by summing the iron X-Ray map and the Cumulative 6 binary image (Table 1; see explanation below). This image was then thresholded to segment the light coloured areas representing remaining minerals containing iron. An inverted binary image of the thresholded area was then produced as in Fig. 7b. Any image can be inverted by the *Edit->Invert* command which applies a (Maximum Greyscale

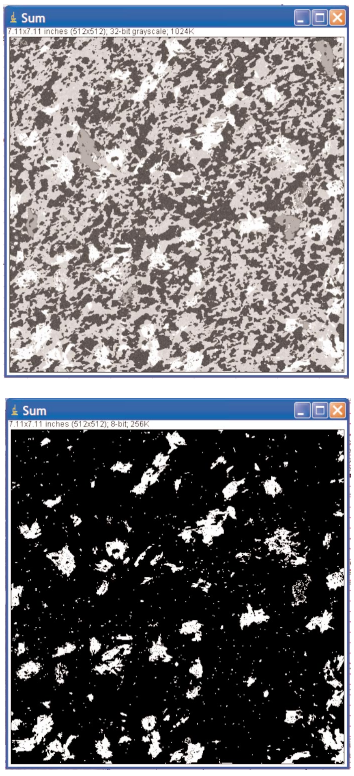


Fig. 7. a) Image created by using the *Image->Stack-> Z Project ->Sum Slices* command on a stack consisting of the iron X-Ray map and a binary image in which all minerals previously measured, including ilmenite, are black. b) An image in which all the high iron areas are white, made by thresholding the high iron areas of a), converting the thresholded image into a binary map, and then inverting the binary map with the *Edit->Invert* command.

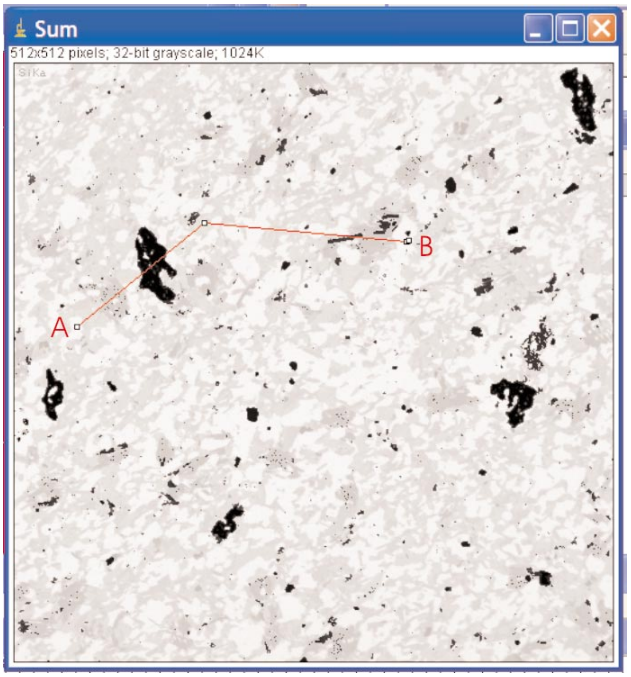


Fig. 8. Image created by using the Image->Stack-> Z Project ->Sum Slices command on a stack consisting of the silicon X-Ray map and a binary image in which all minerals that had previously been measured are black. Previously measured minerals show as dark grey to black; quartz is very light grey; other minerals are various shades of medium grey. The red line, drawn with the segmented line tool, is the line of profile shown in Fig. 9.

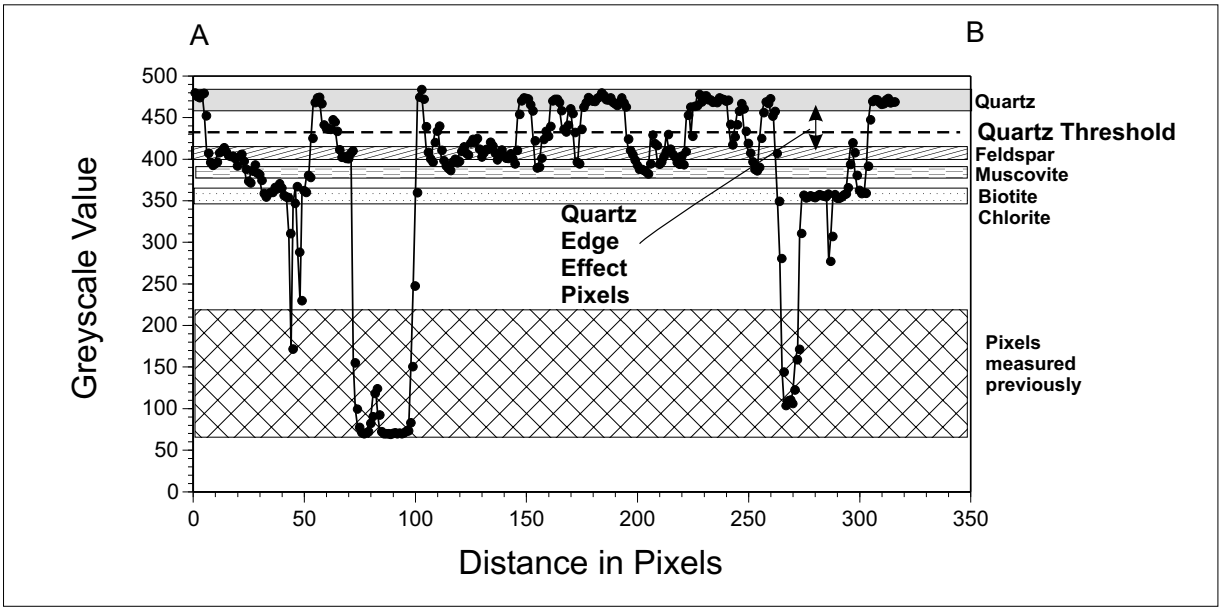


Fig. 9. Greyscale profile along the red line shown in Fig. 8 replotted from the text data of the *Analyse-Plot Profile* command of *ImageJ*. The greyscale ranges of quartz, other minerals and previously measured minerals are as indicated. The white areas are edge effect pixels. A threshold value for quartz is chosen so as to approximately apportion quartz edge effect pixels between quartz and other minerals.

Value of image)-(Pixel Grey Scale Value) conversion to each pixel in the image. This inverted image can then be used as one or more of the slices in a stack to suppress the greyscale values of all minerals except those of interest, in much the same way as the "Cumulative" images are used to eliminate minerals that have already been measured (see below).

2.3. Thresholding the image to select only the mineral of interest.

The image to be thresholded may be a single X-Ray map or a composite image made by combining any number of X-Ray maps via the *Image->Stack->Convert Images to Stack* and the *Image->Stack-> Z Project ->Sum Slices* commands. Incorporation of a backscatter image into the stack can be useful for more precisely demarcating mineral boundaries in some cases. For example, to measure quartz in the example here, a stack is made consisting of the silicon X-Ray map and a binary image in which all minerals that had previously been measured are black (in this case, monazite, apatitite, pyrrhotite, rutile, titanite, ilmenite as per Table 1), and then another image is created (Fig. 8) by adding together the greyscale values of corresponding pixels via the *Image->Stack-> Z Project ->Sum* command.

2.3.1. Choosing the threshold value.

For greyscale segmentation, the only viable method of attributing edge effect pixels is to equally apportion them between the mineral of interest and all other minerals. This will probably tend to minimize the area of the mineral being measured, but the error is acceptably small (see Lydon & Hunt, 2005). Deciding threshold values can be done by one or a combination of three different approaches:

*i) By inspection of a profile of grey scale values across the imag*e.

Select the line, segmented line, or freehand tool from the Menu Bar and draw a line on the image so that it passes through one or more of the lightest coloured areas (the mineral grains of interest) as in Fig. 8. This line defines the line of profile through the image. Select *Analyse->Plot Profile* and a profile window will appear showing a profile of greyscale intensity along the line (Fig.9). Identify the maximum value of greyscale shown by the mineral of interest and set this value as the upper threshold limit on the Threshold Histogram (see below). Identify the plateau range of the mineral of interest (relatively flat parts of the profile

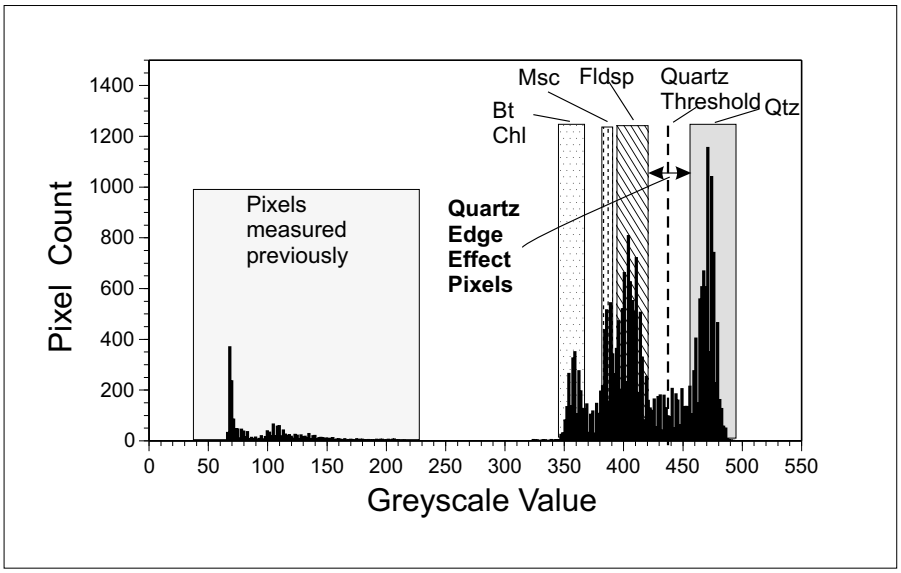


Fig. 10. Histogram of the greyscale values of the image shown in Fig. 7 replotted from the text data of the *Analyse-Histogram* command of *ImageJ*. The "greyscale" ranges of quartz, other minerals and previously measured minerals are as indicated. The white areas are edge effect pixels. A threshold value for quartz is chosen so as to approximately apportion quartz edge effect pixels between quartz and other minerals. Note "greyscale value" is the sum of the greyscale values of the two images used in the stack from which this histogram was created.

where it passes across grains of the mineral of interest. Identify the maximum plateau value of the surrounding background area of the image area (in this case the upper limit for feldspar). Set the lower threshold value as about half way between the plateau value and the lower limit of the plateau range of the mineral of interest.

*ii) By inspection of a histogram of grey scale values of the entire imag*e.

A histogram of the entire image to be segmented is obtained by selecting the "Sum" image and applying the *Analyze->Histogram* command. It should be noted that all *Analyze* commands works only on the thresholded part of the image if the *Image->Adjust Threshold* command has been applied. The greyscale values are those resulting from the *Sum Slices* command, but these may be reset to a 0-255 range by thresholding the entire image, clicking the "Apply" button, and deselecting all options in the "Apply LUT" window (the default LUT is a linear function of greyscale to a 1-255 range). The most appropriate threshold value for the mineral of interest is set at the frequency distribution inflection between the slope of diminishing response from the mineral of interest at the high end of the greyscale values and the slope of increasing response of other minerals. As in Fig. 10, the point of the inflection in the histogram may be somewhat arbitrary, and so the recourse is to choose the threshold half way between the lower limit of the mineral of interest and the upper limit of the remaining populations, that it divides the edge effect pixels of the mineral of interest approximately equally between the two.

iii. By adjusting the lower threshold limit to just avoid random speckling.

Adjustment of the lower threshold value (see below) dilates or erodes the highlighted mineral

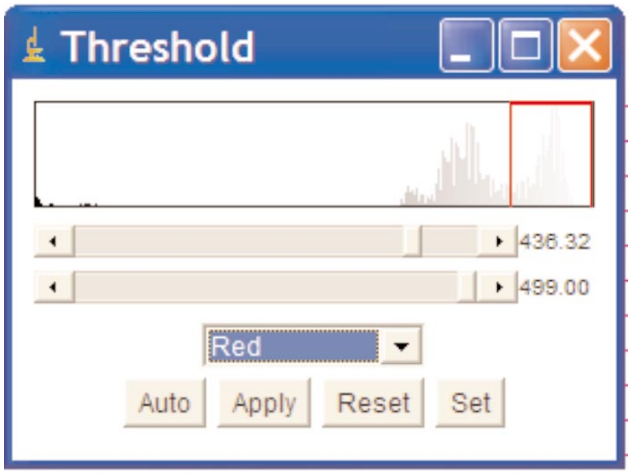


Fig. 11. The Threshold window in ImageJ. The threshold values are adjusted by moving the sliders for the lower limit (upper slider) and upper limit (lower slider) to the values desired. The values at the end of the bar indicate the greyscale value currently selected.

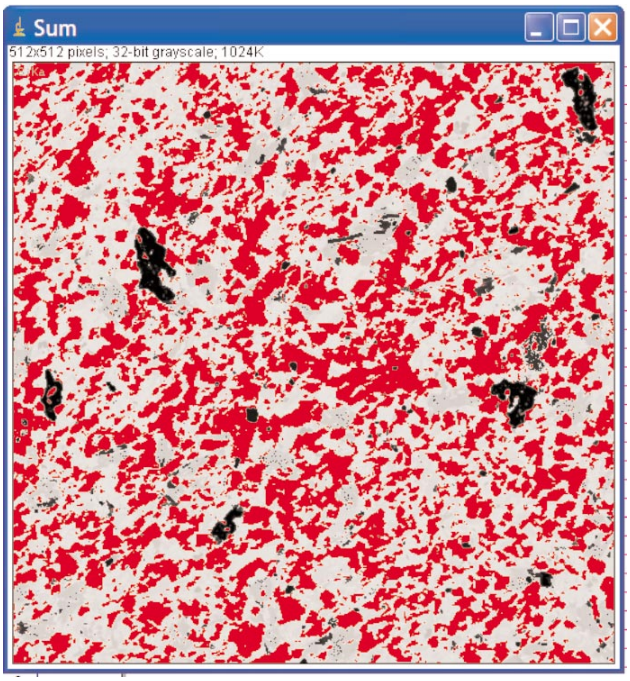


Fig. 12. The image of Fig. 7 thresholded so that areas with a "greyscale" value of >436 (Fig. 10) appear as red.

grains of interest. Lowering the lower threshold value cause dilation to the point that pixels of other minerals start to become highlighted, causing a speckling over the image area. Because the majority of edge effect pixels occur at the edges of mineral grains (Fig. 33), an appropriate threshold value is one that achieves maximum dilation of the mineral grains of interest without significant speckling in other minerals.

2.3.2. Thresholding the image.

With the image to be thresholded selected, click *Image->Adjust->Threshold*. The "Threshold" window that appears (Fig. 11) shows a histogram of the grey levels of the image, underneath of which are two sliding bars. The upper sliding bar adjusts the lower limit of the threshold; the lower bar adjusts the upper limit of the threshold. In the drop down menu there are three choices of how you would like the thresholded area to be displayed on the image. The "Red" (thresholded area coloured red) and the "Over Under" (thresholded area in greyscale; the area under the threshold coloured blue; the area over the threshold coloured green) options are the most satisfactory. The sliding bars are then adjusted to capture the threshold range decided in the steps above. The thresholding operation should be monitored in the image area

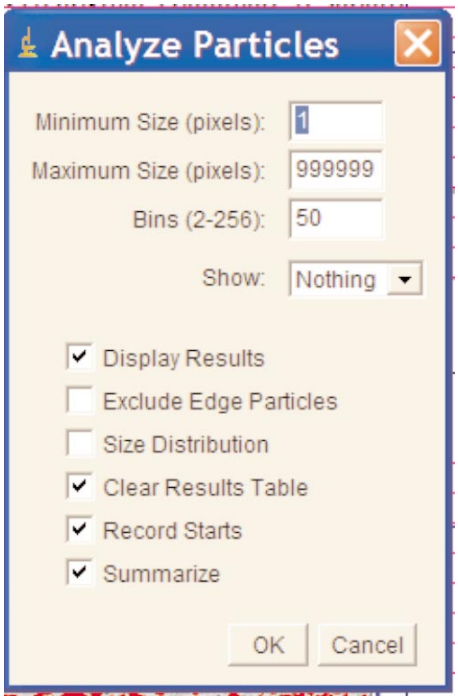


Fig. 13. The "Analyze Particles" window showing the recommended selections.

(Fig. 12) to make sure that the thresholding values chosen are satisfactory.

2.4. Measuring the thresholded areas of the image

The area of the thresholded parts of the image area is measured by selecting the thresholded image and applying the *Analyze->Measure* or *Analyze->Analyze particles* command. The latter causes an "Analyze Particles" window to appear (Fig. 13). Check the "Display results", "Clear Results Table", and "Summarize" options, and select "Nothing" from the drop down menu, and accept the default Minimum Size of 1 and Maximum Size of 999999 as in Fig. 13 . For the *Analyze* command, options are set via the *Analyze->Set Measurements* command, which causes a "Set Measurements" to appear (Fig. 14). Set options as per Fig. 14.

The important result from the Analyze Particles command appear in the Summary window (Fig. 15), which can be copied and pasted into another application as a record. Of main interest is the "Total Area" (expressed as number of pixels) and the "Area Fraction", which give an immediate result for the mineral of interest. The "Results" window (Fig. 16) records the parameters asked for in the "Set Measurements" window as tab separat-

ed text, which can be pasted directly into a spreadsheet for later complation.

2.5. Eliminating measured areas from the image so that they will not be incorporated into subsequent measurements.

Elimination of areas that have been measured is done by adding the measured area to a cumulative binary black/white image in which measured areas are black and umnmeasured areas are white. One or more copies of this cumulative image is then used as slice(s) in a stack along with the appropriate X-Ray maps to segment the next mineral. These Cumulative Images serve to darken areas which already have been measured and remove them from the greyscale range of the mineral to be segmented.

i) Make a binary image of a mineral distribution.

This done immdediately after measuring a thresholded area as in the step above. With the thresholded image selected, apply the *Process->Binary->Threshold* command. Alternatively one can click on the "Apply" button in the Threshold window, and check off all the options in the "Apply LUT" window that appears (Fig. 17). Make sure that the Foreground is set to black and the Background is set to white (use *Edit->Options->Foreground Color* and *Edit->Options->Background Color* to do this) and that the Lookup Table in use is a linear correlation of greyscale colour to a 0-255 range.

ii) *Save the binary image.*

iii) *Close all other image windows.*

This is needed to prevent a possible program error alert or accidentally combining unwanted images in the cumulative image.

iv) *Open the last saved Cumulative Image*

v) Make a stack of the mineral binary image just created and the Cumulative Image just opened.

vi) Create a new Cumulative Image.

This is done by using the *Stack->Z Project->Min Intensity* command or alternatively using the *Stack->Z Project->Sum Slices* command, thresholding the image to exclude white areas, then

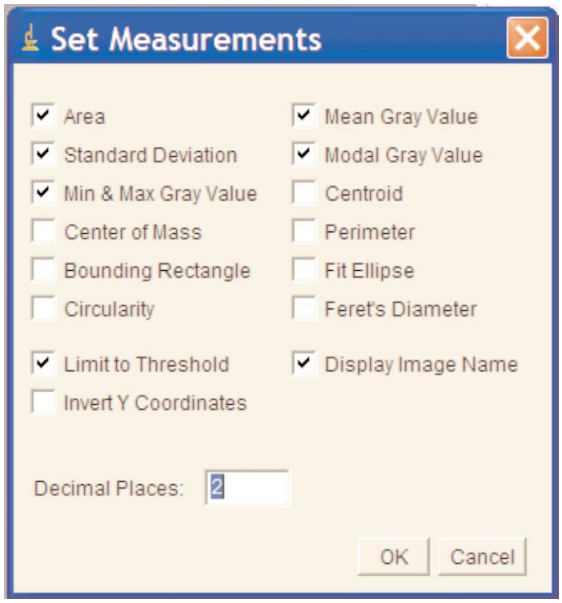


Fig. 14. The "Set Measurements" window showing the recommended selections.

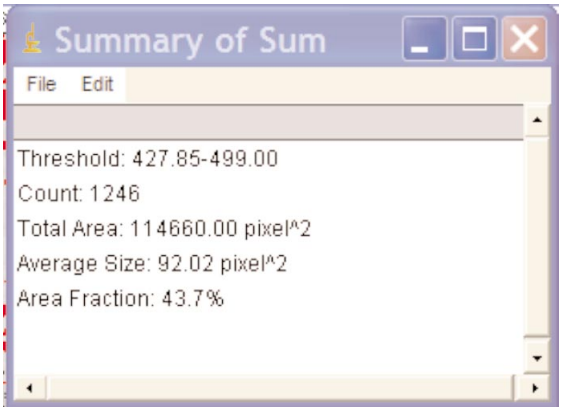


Fig. 15. The Summary window that summarizes the results of the Analyze Particles command, if "Summarize is checked in the Analyze Particles window (Fig.12).

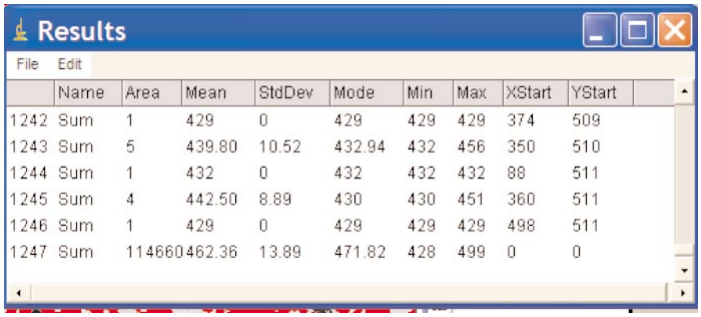


Fig. 16. The Results window that lists the results of the *Measure* and *Analyze Particles* commands. The last entry is that from the *Analyze->Measure* command, whereas all previous entries are from the *Analyze->Analyze Particles* command. Any row may be selected and copied into a spreadsheet.

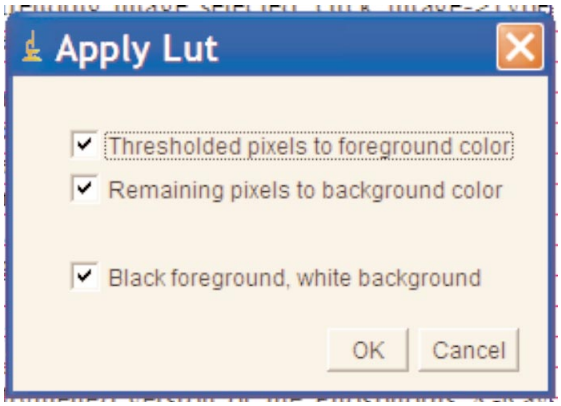


Fig. 17. The "Apply LUT" window showing options required for conversion of a thresholded image to a binary image.

using the *Process->Binary* command.

vii). Save the new Cumulative Image.

2.6. Producing a table of results and a mineral distribution map.

i). Complete measurements for all minerals

Repeat Steps 3, 4 and 5, until all the minerals are accounted for. Don't forget at some stage to threshold and measure the area occupied by any text in the images as the element identifier in top left-hand corner in the current exampleAn inve

ii)Check the chemical composition of unclassified pixels.

Make an inverted image of the last saved cumulative map, so that unclassified pixels are black and areas which have been classified are white. Save this file into the computer folder or sub-directory that has only the X-Ray maps, and then make a stack of all these images using the *File-Import-Image Sequence* command. Scroll the stack to the inverted cumulative and check the chemical composition of unclassified pixels by selecting these pixels with the rectangle select tool and the *Image->Stacks->Plot Z-axis Profile* as described in Section 1.v. above. Scattered single pixels can be ignored as random pixels that fell through the classification procedure, but attention should be given to contiguous unclassified pixels, because they may represent unrecognized minor minerals. If this is the case, then consideration should be given to repeating the analysis from the point where other grains of this mineral may have been erroneously segmented with another. For this reason, it is advisable to retain copies of all the Cumulative Images and numbering them as in Table 1.

ii) Make a greyscale mineral distribution map.

This involves making a greyscale version of all the binary *<mineral name>.tif* files saved in Step 5.i. above and then combining all the greyscale images so that each mineral has its own greyscale value. First, one has to decide the greyscale value desired for each mineral in the final greyscale mineral distribution map, as for example in Table 2. The greyscale value of the area covered by a mineral in a *<mineral name>.tif* image is zero (black). To convert it to the desired grey scale value, open the binary *<mineral name>.tif* image and use the *Process->Math->Add* command to add the grey scale value desired. Black pixels are converted to the greyscale value (0 + x = x, where x is the greyscale value) but white areas remain white (255 + x = 255, because 255 is the maximum number allowed). Repeat for all the *<mineral name>.tif* images and then combine them using the *Image->Convert to Stack* and *Image->Z Project->Min Intensity* commands. The resulting greyscale minerals distribution map will have the greyscale values as desired.

Mineral	Greyscale Value
Not Classified	0
Label	255
Iron sulphide	60
Ilmenite	120
Calcite	160
Titanite	200
Monazite	70
Biotite	180
Apatite	100
Chlorite	170
Rutile	100
Muscovite	190
Epidote	110
Feldspar	210
Quartz	240

Table 2. List of minerals in image area and greyscale values to be assigned to them.

A table can be constructed in the spreadsheet by combining the data separately pasted from the "Results" text window in Step 4 above. The pixel count is converted to area % by dividing by the number of pixels in the image (in this case 262,144) and multiplying by 100.

2.7. Converting the greyscale image to a coloured image.

For display purposes, the greyscale mineral distribution map is not very informative if the map contains more than four or five minerals. The eye cannot distinguish more than this number of different shades of grey in a mosaic (Fig. 18). This greyscale mineral distribution map can be rendered in colour by replacing the grey shades with an appropriate colour. This is most efficiently done by using a "Replace Colour" routine of a photo-editing application.

Mineral class	Area %
Quartz	43.68
Feld	18.72
Muscovite	22.27
Biotite	3.7
Chlorite	5.81
Ilmenite	1.54
Titanite	0.61
Apatite	0.53
Epidote	0.33
FeS	0.03
Rutile	0.06
Calcite	0.66
Text (of upper left hand corner)	0.22
Total	98.16

Table 3. A modal mineralogical analysis of Fig. 18 produced by the greyscale segmentation method using *ImageJ*..

Fig. 18. Greyscale mineral map produced by greyscale segmentation of 10 X-Ray maps (Al, Ca, Fe, K, Mg, Na, P, S, Si, Ti) using *ImageJ*.

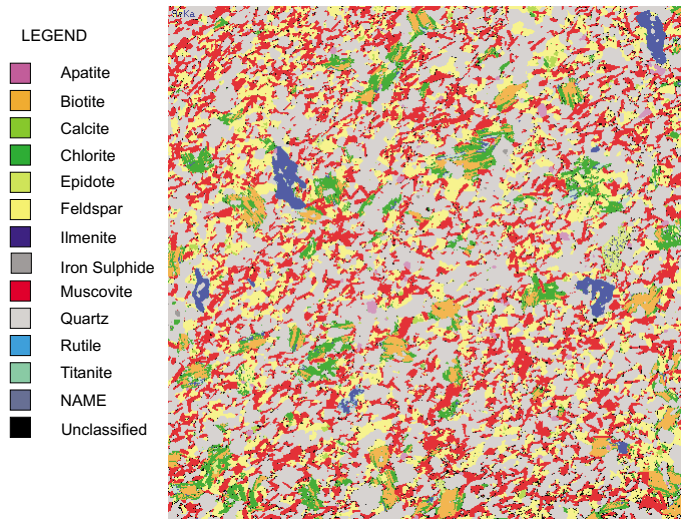


Fig. 19. Coloured mineral map produced by colour replacement of greyscale values of image in Fig. 18.

3. MODAL MINERALOGICAL ANALYSIS USING *MULTISPEC©*

3. Introduction

Multispec© works by carrying out mathematical manipulations on a series of bitmaps representing different information (channels) of the same area. The overlaid images are contained in a multispectral image file with a .*.*lan* extention. Manipulations may be carried out on any number or combination of these channels by selecting the channels of interest within the program. In the present case, each channel is a 512 x 512 pixel greyscale X-Ray map of a fine-grained rock slice. An X-Ray map show the distribution and relative abundance of a given element. The value of each pixel varies from 0 (black, zero abundance) to 255 (white, maximum abundance).

Multispec allows basically two methods of dividing the image into areas of similar multi-channel characteristics (i.e. minerals with the same chemical compositions):

A) An unsupervised cluster analysis in which the program calculates the groupings; and

B) a supervised classification based on user-defined training sets.

Multispec© and its algorithms are well described in the documentation (Landgrebe, D. and Biehl, 1991-2002) that can be down loaded with the application, and are not described here. This report is intended only as a "quick-start" guide to those who want to quickly carry out a modal mineralogical analysis from a set of X-Ray maps.

The general procedure for a complete modal mineralogical analysis of the sample using Multispec© involves:

1) combining the separate X-Ray maps (**.tif* files), into a single multispectral (**.lan*) file;
2) gaining familiarity with the range of minerals in the sample;
3) choosing a method of analysis;
4a) carrying out an unsupervised cluster analysis;
4b) assigning edge effect pixels to a mineral class;
5a) selecting training fields for each mineral class;
5b) choosing the classification method for mapping the mineral classes;.
6) Producing a table of results and a mineral distribution map.

3.1. Convert the different X-Ray maps (*.tif files) into a multispectral file.

1.i) Open the first X-Ray map.

Note that the X-Ray maps used here are *.tif files of 512 x 512 pixels with a 0-255 grey-scale value. This is the most common format for X-Ray maps and it is assumed that this is the image format for all operations described here. The greyscale value of a pixel is proportional to the number of X-Ray counts collected at that beam position for the element, the proportionality being set by the SEM operator (see Section 1, pages 1-3).

For convenience of later easy reference, write down the order in which the different element X-Ray maps are opened, because these will be the

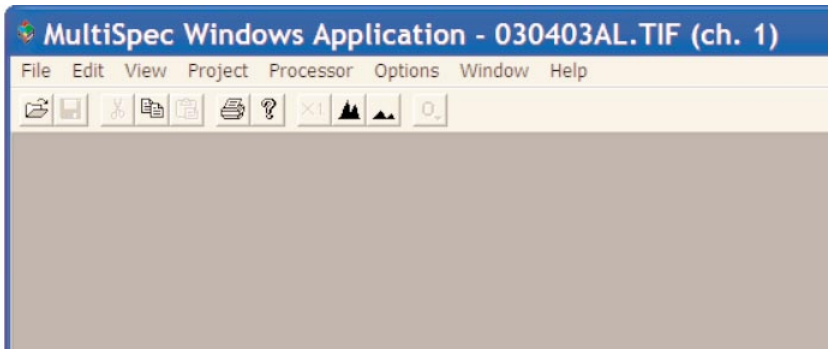


Fig. 21. The main menu bar of *Multispec©*. In this article, the first-listed command of command chains written in italics refers to selection from this menu. Note that the buttons second and third from the right are zoom controls for the active image window.

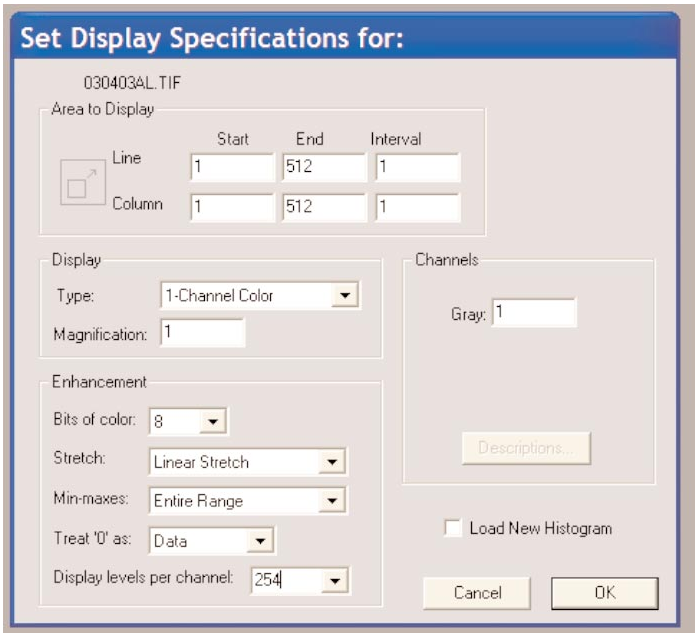
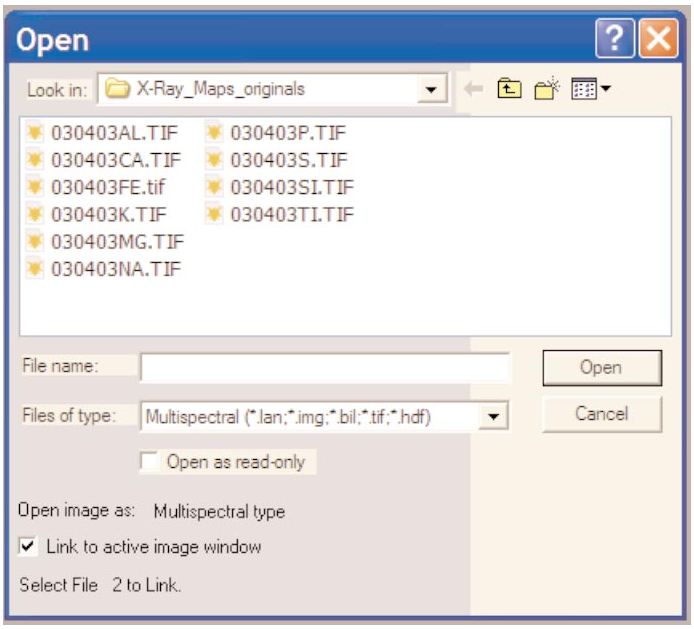


Fig. 22. The Set Display Specifications for: window which appears after opening the first X-Ray map.



"Fig. 23. The "Open window which appears after using the *File->Open* command. The "Link to active image window" option appears only if an image file has already been opened. To link subsequently opened files to the first file, select this option.

Channel numbers used by the software i.e. the first map opened will be Channel 1; the second X-Ray map opened will be Channel 2; and so on.

Open the first image by *File-> Open Image* (point to first *.tif file in the series of images) -> *Open*

A "Set Display Specifications for: (filename)" will appear (Fig. 22). Most of the default values will probably be satisfactory but make sure that they are all as in Fig.22:

Area to display: This information is read off the header for the *.tif file (in this case 512 x 512 pixels). Check that both line and column start with 1, end with 512 and an interval of 1. This will display the entire image. Check that all successive images have these same values.

Display type: 1 channel color (i.e. only one greyscale colour channel for the image)

Magnification: 1 (will display entire image in the image window).

Enhancement: 8 bits of color

Stretch: Linear Stretch . This causes the grey scale intervals to be equally spaced over the range. Equal area stretch causes the grey scale intervals to be set so that each interval represents the same number of pixels and provides the maximum contrast to the image.

Min-Maxes: These are options to select the beginning and end points of the image histogram used in display enhancement. Set to "Entire Range" because clipping the data is not desired..

Treat "0" as: Data.

Display levels per channel: 254 (for 8 bit data)

1.ii) Open the second image of the series of X-Ray maps to be overlaid.

Use *File -> Open Image* again. The directory from which the first image file was loaded will automatically open as in Fig. 23.

Check the "Link to active image window" box.

"Select File 2 to link" will appear in bottom left hand corner of dialogue box.

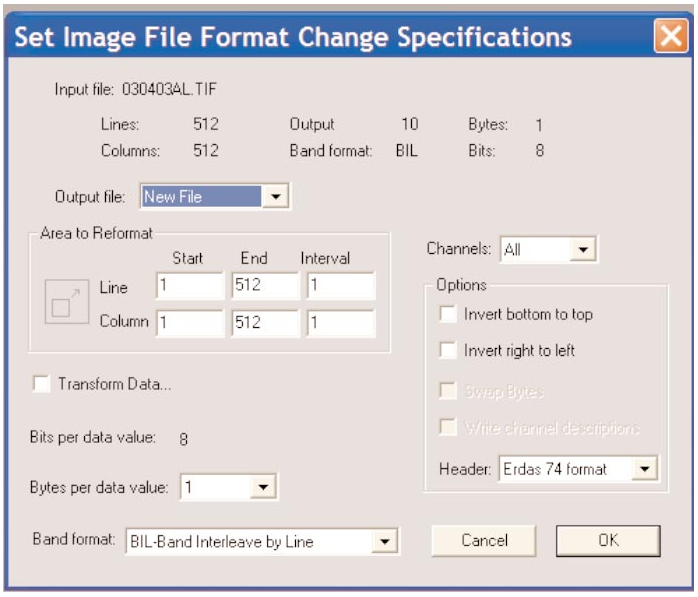


Fig. 24. The "Set Image File Format Change Specifications" window which opens on using the *Processor->Reformat->Change Image File Format* command.

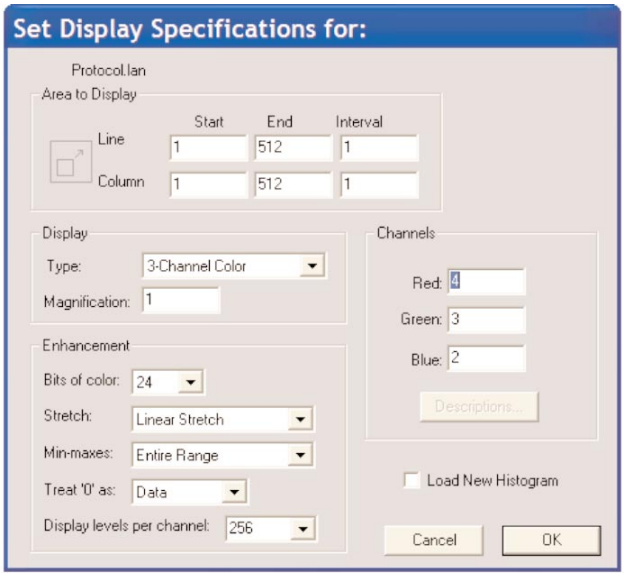


Fig. 25. The "Set Display Specifications for: window" which appears after opening a *.lan image or applying the *Processor-Display Image* command with a **.lan* image selected. This window is exactly the same as in Fig. 22, except that with a *Display Type* of "3 Channel Color" selected, the Channels box requires entry of the choice of channels (X-Ray Maps) to be displayed as Red, Green and Blue for display of an RGB image (see Fig. 26.

Click on the second *.tif file in the series of images.and "Open".

1.iii) Open remaining X-Ray maps.

The "Open" window will automatically open at the directory from which the first two files were loaded. Repeat selecting the files in the order that the channels are wanted. After the last file has been opened click "Cancel". If you wish, you can save this file as a multi-page *tif file.

*1.iv) Convert the multi-page *.tif file into a multi-spectral file.*

Use the *Processor -> Reformat -> Change Image File Format* and a "Set Image File Format Specifications window will appear. If the default values are not as in Fig 24 then change them accordingly:

Output: New file

Channels: All

Area to Reformat: Start 1 End: 512 Interval: 1 for both *Lines* and *Columns*

No *Tanform* or *Inversions*.

Header: Erdas 74 format

Bytes per data value: 1

Band Format: BIL-Band Interleaved by Line.

Click O.K.

Name the file (with a **.lan* extention)

3.2. Inspect set of X-Ray maps to gain familiarity with distribution of different minerals

This second step is required for both the cluster analysis and the training area methods. The number of different minerals in the image area is needed to guide the user in choosing the number of classes for a cluster analysis method. Knowing the distribution of the different minerals is essential to choosing the training areas for the training fields method. A knowledge of the range of minerals in the sample is best acquired through prior petrographic study. As with *ImageJ*, the two best techniques for examining the distribution of minerals in the image area is via an RGB projection of three X-Ray maps and via a profile of the average greyscale value of all elements in a selected small part of the image area.

It should be noted here that *Mutispec*© logs all operations in a "Text Output" window which provides a very convenient record of an analysis session. The results of operations can also be option-

ally recorded in this text window (which can later be saved as a text file) and/or saved directly to a computer file. The text window display is very useful for copying and pasting results into graphics software applications for custom display of the results.

2.i). *Create a two or three element RGB map of the image area*.

Open the *.lan file that was just created. A "Set Display Specifications for:" window will appear (Fig. 25). Set the options as in Fig. 25 i.e.:

Area to display : to see the entire image Start 1 End: 512 Interval: 1 for both Lines and Columns.

Display Type: 3-Channel colour (the other options are for two colour or 1 colour grey scale display).

Channels: Set the Red, Green, and blue Channels to the channels o(X-Ray maps) of your choice. The sequential list that was written down earlier is the easiest reference to which channels represent what channels. Channel colours can easily be reassigned later.

Bits of colour: 24

Stretch: Linear Stretch

Min-maxes: Entire Image

Treat "0" as: Data

Display levels per channel: 256

Click on "Load new Histogram" if this option is not greyed out. When loading a new histogram a "Set Histogram Specifications" window will appear. Set the values to:

Method: Compute new histogram

Area to Histogram: Start 1 End: 512 Interval: 1 for both Lines and Columns.

Channels: All

Click on *"List histogram summary"* - this will write the histogram data to the text output window and can be saved for future use.

An image of the X-Ray maps will be displayed, false-coloured by the selected channels. Different minerals will have different colours. For example, a yellow colour will indicate about equal contributions from the red and green channels.

Explore different combinations of channels by using the *Processor ->Display Image* command which will open the "Set Display Specifications for" window as in Fig. 25. Select the different channels for the three colours, click O.K.and a dif-

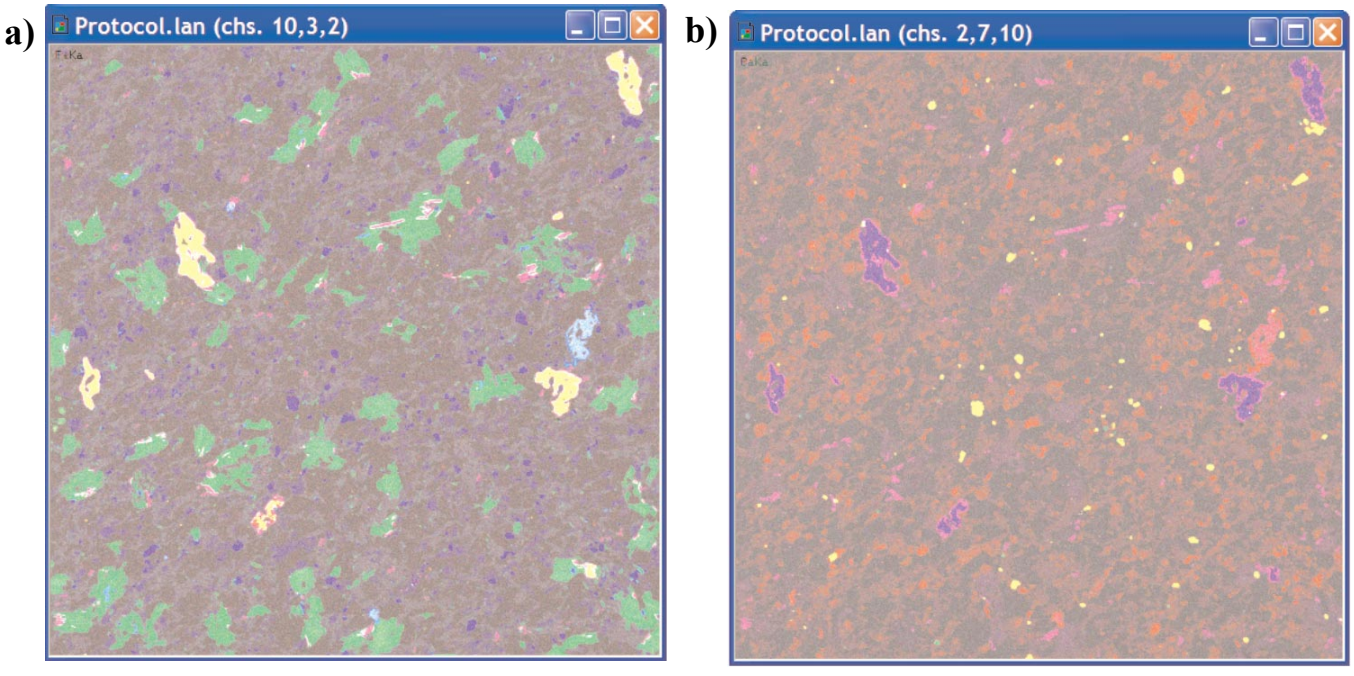


Fig. 26. A three colour display for:
a) Ti (red), Fe (green) and Ca (blue) to distinguish the different titanium-bearing minerals. Ilmenite is yellow; titanite is magenta to white (because it replaces and interdigitates with ilmenite), rutile is red. Epidote is distinguished as turquoise. The green areas are chlorite and biotite. Apatite and calcite are the clearer blue areas.
b) Ca (red), P (green) and Ti (blue) to highlight the distribution of apatite (yellow) and monazite (green). The different titanium-bearing minerals are blue to magenta. Epidote and calcite are red.

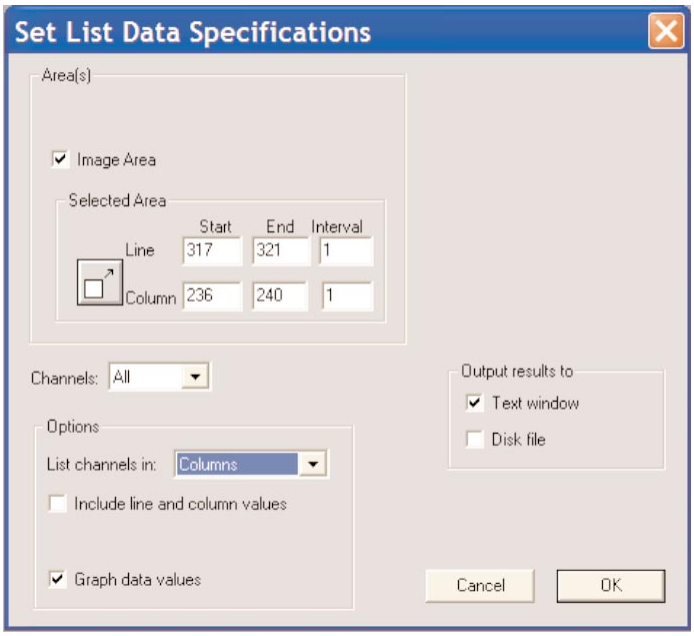


Fig. 27. The "Set List Data Specifications" window which opens on using the *Processor->List Data* command.

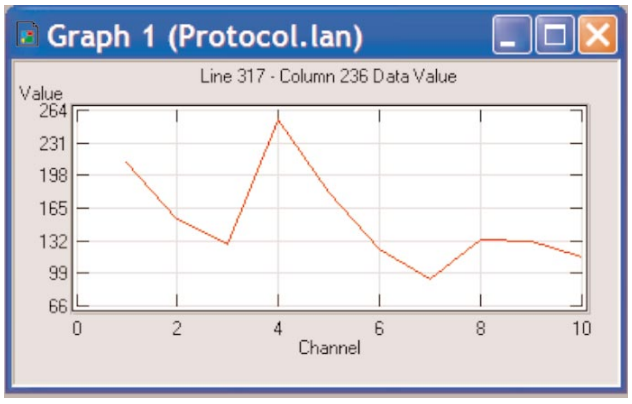
ferently coloured image will appear accentuating different minerals (Fig. 26 and 27). By repetitive changing of the channels, a familiarity of the distribution of the different minerals should be gained, as well as a knowledge of which combination of colours best accentuates which mineral.

Note that this inspection of coloured images can equally as well be carried out on the multi-paged **.tif* file created in 1.iii above. During familiarization with mineral distributions in the image area, it is a good idea to save an RGB image that identifies the distribution of a specific mineral for later reference to facilitate choice of training fields and assignment of cluster classes to mineral species.

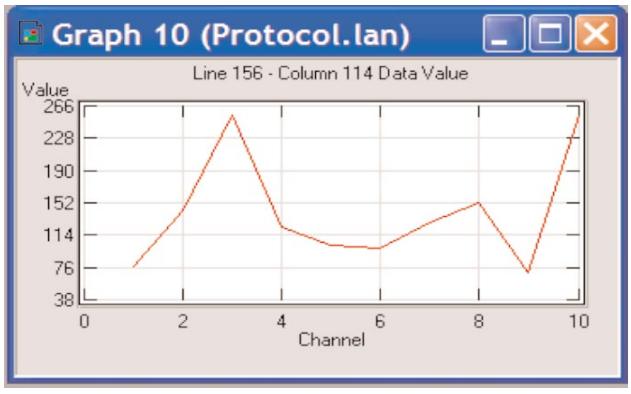
2.ii. Create a multi-channel profile of a small area of the image.

A profile of the greyscale value of all channels of a selected pixel is also useful in identifying all the chemical constituents, and hence an identification of a specific mineral. This is done by selecting a small area of the mineral of interest by dragging the cursor across the **.lan* image. Apply the *Processor->List Data* command, and a "Set List Data Specifications" window appears (Fig. 27). Select the "Graph data values" option. The greyscale values for all channels for each pixel in the selected area is listed in the Text window. The values that are graphed (Fig. 28) are only for the pixel in the upper left hand corner of the selected area. If a graph of the average greyscale values for each channel of all the pixels in the selected area is required, then this is most rapidly done by using the *Window->New Selection Graph* command Fig. 29).

In interpreting the profile, it should be remembered that the greyscale values for most X-Ray maps are not uniformly calibrated against content of the element in the mineral. Usually individual maps are calibrated such that the maximum content of the element in the image area has a greyscale approaching 255 (white). Thus the relative greyscale values of the different elements do not indicate the relative proportions of the element is in the mineral. For example, in Fig. 28 (a profile



a) MUSCOVITE



b) ILMENITE

Fig. 28. A multi-element (channel) profile of a pixel of a) muscovite and b) ilmenite obtained using the *Processor->List Data* command with the "Graph data values" option.

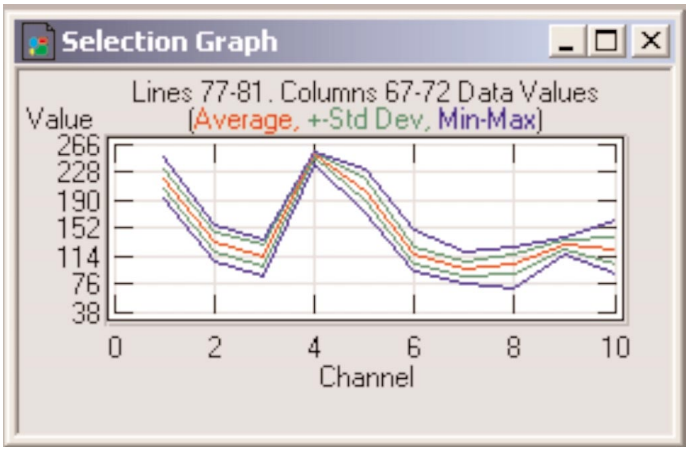


Fig. 29 The "Selection Graph" window which opens on using the *Wndow->New Selection Graph* command on a selected area of a **.lan* multichannel image. In this example a small area of muscovite was selected. The location of the area is given as Lines and Columns measurements.

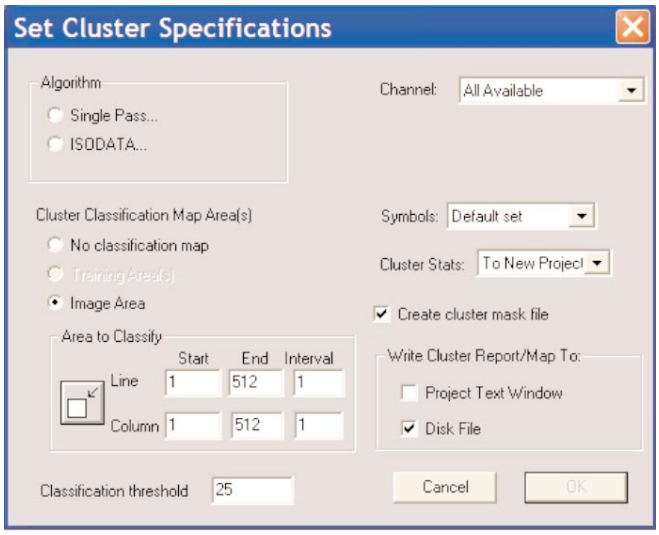


Fig. 30. The "Set Cluster Specifications" window which opens on using the *Processor->Cluster* command.

for a muscovite pixel) it is intuitive that the mineral has high contents of aluminum (channel 1) and potassium (channel 4), but it is not obvious that the mineral also has a major content of silicon (channel 9). The relatively high silicon content is only appreciated by comparing the profile of muscovite with that of a mineral that does not contain silicon, such as ilmenite in Fig. 29.

3.3. Choose a method of analysis.

After a list of minerals present in the image area has been compiled, the next step is to choose the method by which the modal mineralogical analysis is to be carried out. Basically, there are two options. If one is not confident that all the minerals in the image area have been identified, then it is better to choose an unsupervised cluster analysis method, which has a chance of identifying unrecognized mineral classes. If one is satisfied that all minerals have been identified and that one knows where some example grains occur in the image area, then it is best to choose the supervised training field method.

3.4. Unsupervised cluster analysis.

With the **.lan* image window active (i.e. selected so that the title bar is dark blue) apply the *Processor->Cluster* command. A "Set Cluster Specifications" window will appear (Fig. 30).

4.a. Choose cluster analysis algorithm.

There are two choices for the clustering algorithm method, which later on lead to different choices from different windows. The "Algorithm" frame is described on p. 21. The remaining frames apply, irrespective of the choice of "Algorithm". Set the following choices:

Cluster Classification Map Area(s). Select Image area. This will produce a map of the entire image area false-coloured according to the classification calculated by the cluster analysis.

Area to classify: accept default values for entire image (all 512 lines and 512 columns starting at 1 with an interval of 1)

Classification threshold: Set to 25. This parameter determines the maximum Euclidian distance of a pixel from the nearest final cluster centers for inclusion in that cluster. If the pixel is too far away from the nearest cluster center , it is blanked out on the **.clu* map (see below). A classification threshold of about 25 has been found to be the optimal value for the X-Ray maps analysed here.

Channel: All available.

Symbols: Default Set

Cluster Stats: To New Project

Create Cluster Mask File: Check this option which will produce a cluster map (**.gis*) file that shows all pixels i.e. it ignores the classification threshold and assigns each pixel to the nearest cluster center.

Write Cluster Report/Map to: Check "Disk File" which will produce a cluster map (**.clu*) file in which pixels which lie at a greater Euclidian distance than the classification threshold are blanked

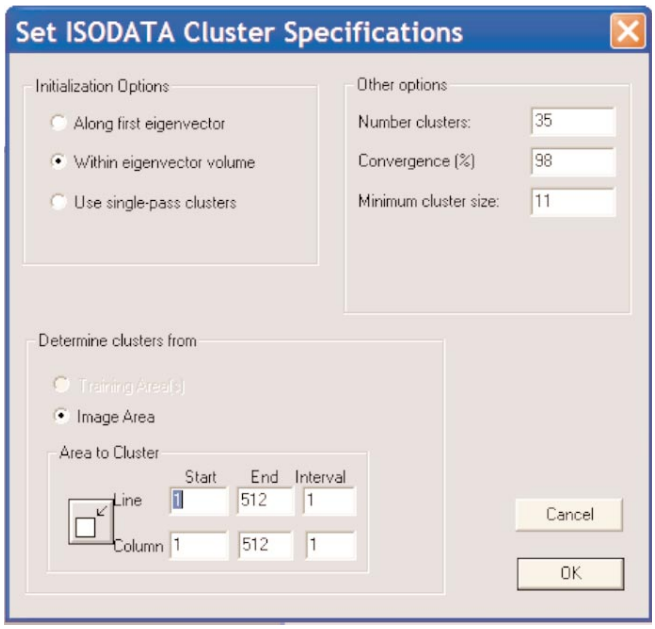


Fig. 31. The “Set ISODATA Specifications” window which opens on selecting ISODATA in the “Set Cluster Specifications” window (Fig. 30).

out, but is otherwise identical to the **.gis* file mentioned above. Comparison of the **.gis* and **.clu* maps gives an indication of what mineral grains or parts of a mineral grain depart most from the compositional range defined by a cluster class. Do not check "Project Text Window" because the output will swamp the Text Output File. The text report consists of a matrix of the map area in which each pixel is represented by a text character coded to the cluster analysis class (number of lines = number of lines in data set; number of characters per line = number of rows in data set). In the present application, there is little use for the text report, except perhaps to use a text editor to search for the locations of a particular class.

Algorithm:

"ISODATA” As explained by the Multispec© manual the Isodata method of cluster analysis starts with a pre-determined initial set of clusters, the number of which are set by the user. As mentioned above, this number should be about three times the number of mineral phases known to be present in the sample. After determining the centre of each cluster, the algorithm then associates each pixel of the image area with the cluster whose centre is the smallest Euclidian distance from the pixel. After all pixels have been assigned to a cluster, a new centre for each cluster is calculated and the process of assigning pixels to the new set of clusters is repeated through another iteration. The iterations are stopped when the percentage of pixels that are not reassigned to a different cluster exceed the Convergence value (commonly 98%) set by the user. Clusters containing fewer pixels than the Minimum Cluster Size parameter set by the user are eliminated. At a convergence value of 98%, the results are highly dependent on the initial clusters. The higher the convergence value, the longer the computation time.

On selecting “ISODATA” a "Set ISODAT cluster Specifications" window will appear Fig. 31).

Initialization options

There are three choices for defining the initial clusters for the iterative cluster analysis. The first two are based on Principle Components of the data set:

1. *Along first eigenvector:* The centers of the number of initial clusters, as specified in the "Number clusters" of the "Other options" frame (see below), are equally spaced along the first principal component. The effect of this, in the present case, is to generate classes based on those elements that contribute most to the mineral variability across the sample (K, Mg, Si, Fe in the example used here). If the number of clusters is defined as about equal to the number of minerals in the sample (e.g. 12 in the example here) , the clusters tend to reflect only the most common minerals and edge effects between them. Minor minerals consisting largely of less abundant elements (Ti, P, S) are grouped with the compositionally closest major mineral. In the example here, if the number of clusters is defined as 12, apatite, titanite, pyrrhotite and ilmenite are included in the same cluster, reflecting the low amounts of K and Si in these minerals. On the other hand, among the compositionally-related major minerals, chlorite is distinguished from biotite and Na-rich plagioclase is distinguished from Ca-rich plagioclase.

2. Within eigenvector volume. The number of initial cluster centers are scattered within the volume defined by the first three principal components. The effect of this is to increase the weighting of more elements in the initial clusters, so that a small number of final clusters may distinguish minerals composed of less abundant elements. In the example used here with 12 clusters, a class representing Ca-rich minerals (mainly apatite and titanite) is distinguished, at the expense of losing distinction between chlorite and biotite.

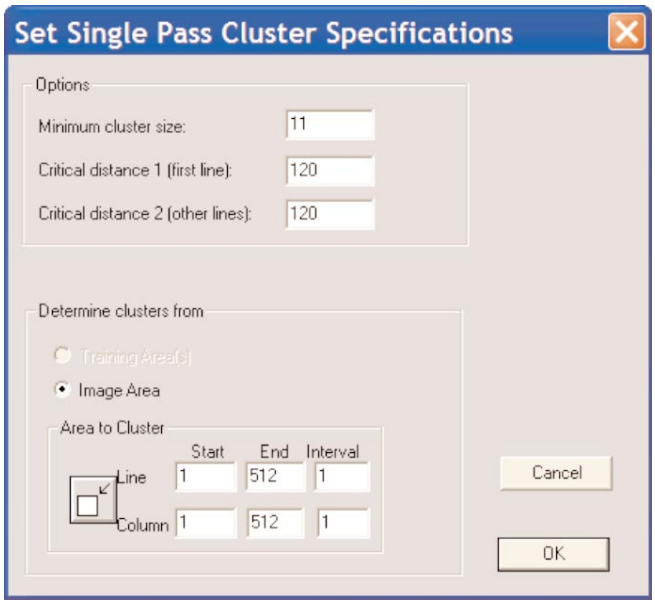


Fig. 32. The "Set Single Pass Cluster Specifications" window which opens on selecting "Single Pass" in the "Set Cluster Specifications" window (Fig. 30).

3. Use single-pass clusters. The isodata algorithm uses the results of a simple one-past clustering to set the initial clusters (see below), and so tends to give a weighting to all elements. Compared to the two methods based on principal components described above, this method gives results that are closer to the "*Within eigenvector volume*" method when number of clusters are about the same.

Number of clusters. (Appears only when the "Within eigenvector volume" or "Along first eigenvector" options are chosen). In order to capture all minerals present, it is recommended that this number be about three times the number of mineral species present within the area of the X-Ray map in order to allow "edge effect" pixels to form their own cluster, which can then be re-attributed proportionally to end member minerals (see below).

Convergence: leave at the default value of 98%

Minimum cluster size. As discussed below, set to between 11 and 50.

Determine clusters from: Select "Image area"

Area to cluster: Make sure that this set to cover the entire image area i.e. Line: Start 1 End 512 Interval 1; Row: Start 1 End 512 Interval 1. If it is not, click on the "expand area" button just to the left of the Line and Column text in the "Area to classify" box.

Algorithm:

Single Pass. This carries out a simple cluster analysis bases on minimum euclidian distances.. In selecting this method a "Set Single Pass cluster specifications" window will appear (Fig. 32)

Minimum cluster size: This determines the minimum number of pixels to constitute a cluster. On the X-Ray maps used here there are 262,144 (512 x 512) pixels. A mineral occupying 0.01% of the image area would therefore theoretically occupy 26 pixels. However, using the default value of 11 is not of much practical importance, because the great majority of clusters end up with >1000 pixels. (Note that the wavelength identifier embedded as text in the pixel image occupies about 70 pixels).

Critical distance 1 (first line): As explained in the Multispec Manual this defines the distance (in data value units) used during the cluster of the first line of each cluster area. If the distance between a pixel and the center of the closest cluster is larger than this value, then this pixel is used as the first pixel to create a new cluster. The distance measure is the Euclidean distance. The smaller the critical distance, the greater the number of classes created. No advantage has been found in treating the first line of data differently from the rest.

Critical distance 2 (other lines): This is the Euclidian distance measure for determining clusters for the other lines. The "Single Pass" algorithm tends to define an excessive number of classes unless the "Critical Distance 2" parameter is set to > 100 to reflect the large radius of the Euclidian cluster resulting from the variation in chemical composition across grains of a single mineral species. For the example used here, setting "Critical distance 1" to 60 and "Critical distance 2" to 120, produced 31 clusters, of which 21 accounted for 99% of the pixels.

No matter what method of cluster analysis is carried out, just before the clustering computation takes place two windows successively appear asking you to save the 1) *.clu (classified image area that also shows thresholded areas) and 2) *.gis file (image area in which all pixels are classified). Records of the cluster analysis that are the most important is the table of class channel means

Cluster	Pixels	%	Channel Means										
			Al	***Ca***	***Fe***	***K***	***Mg***	***Na***	***P***	***S***	***Si***	***Ti***	***Class Name***
			1	2	3	4	5	6	7	8	9	10	
1	420	0.2	146	179.2	250.8	126	193.6	141.5	102.1	115.4	116.8	200	***EDGE_Chlorite/Titanite***
2	72	0	86.7	150	138.3	114.6	97.8	99.7	111.6	128.3	86.9	255	***Rutile***
3	242	0.1	168.9	251.1	115.1	206.7	161	122.3	221.3	113.1	126.2	118.6	***EDGE_Apatite/Musc***
4	1918	0.7	151	152	103.7	110.7	117.1	119.9	106.3	109.6	189.2	142.6	***EDGE_Qtz/Titanite-Apatite***
5	390	0.1	169.4	215.1	118.9	113.8	165.3	190.7	101.2	109.2	144.2	210.4	***EDGE_Titanite/Feldspar***
6	23	0	88.7	251.6	243.6	122.1	105.4	107.6	219.3	132.8	84	253.9	***EDGE_Ilmenite/Titanite***
7	8463	3.2	156.1	127.6	250.9	191.9	209.2	143.2	99.9	113.9	112.9	133.3	***Biotite***
8	26	0	116	255	120.6	135.2	121.9	116.9	241.9	122	111.4	238.1	***EDGE_ApatiteTitanite***
9	63	0	129.2	252	235.6	141.6	168.6	132.8	231	119.1	108	124	***EDGE_Apaite/Biotite***
10	108	0	120.2	123.7	242.3	111.7	108.1	112.8	121.1	224.6	147.3	136.1	***FeS***
11	7889	3	156.7	112.7	144	112.7	137.8	132.8	100.2	109.1	177.9	114.5	***EDGE_Qtz/Chl-Biot***
12	86	0	158.4	135.3	116.6	135.6	143.9	145.9	230.4	137.7	156.5	125.4	***Monazite***
13	696	0.3	184.4	225.9	121.8	220.5	169.7	120.6	102.6	111.5	130.7	204.2	***EDGE_Titanite/Muscovite***
14	1168	0.4	101	254.8	103.9	128.9	108.9	114	251.6	127.9	107.4	118.1	***Apaitite***
15	14	0	173	44.1	70.6	97.5	85.7	18	95	101.3	179.2	92.1	***TEXT2***
16	63	0	111.2	110.8	114.3	108.2	109.2	106.6	87.1	104.8	103.6	101.3	***Unknown***
17	1560	0.6	124.3	248.8	245.4	123.7	140.2	122.9	109.7	123.8	109.1	247.6	***EDGE_Titan/Chl-Ilm***
18	23464	9	184	125.2	108.4	178.2	158.8	131.2	99.3	107.3	161.4	115.8	***EDGE_Musc/Qtz***
19	766	0.3	155.1	249.5	224	120.9	155.9	126.4	109.5	119.1	120.9	144.2	***Epidote***
20	2715	1	81.2	144.7	254.6	121.6	96.5	100.6	114.3	137.1	76	254.5	***Ilmenite***
21	37	0	18	21.3	18	31.5	31.6	28.5	88.5	90.3	18	25.6	***TEXT1***
22	1293	0.5	130	249	131.6	125.4	122.5	115	110	117.3	135.6	253	***Titanite***
23	3540	1.4	147	246.6	103.7	117.9	142.1	155.4	103.7	110.7	128.2	113.1	***Calcite***
24	49385	18.8	184.4	149.8	99.4	109.4	176	209.8	98.4	106.4	154.1	112.6	***Feldspar***
25	14556	5.6	152.8	114.8	250.1	117.3	203.5	149	99.3	112.9	120.7	122.4	***Chlorite***
26	44261	16.9	213.8	135	115.2	244.6	193.4	125.1	98.5	107.6	136.3	120.9	***Muscovite***
27	98903	37.7	149.8	105.7	95.4	100.5	106.1	110.6	102.2	108.8	211.1	111.5	***Quartz***

Table 5. A table of channel means from a cluster analysis copied into a spreadsheet. Text in bold italics were added by the user in the spreadsheet.

which should be copied and pasted into a spreadsheet (Fig.33)

4b. Assign clusters to a mineral class.

No matter what method was used to produce the *.gis or *.clu files, the process of assigning clusters to a mineral species is the same. There are two sources of information to guide the assignment:

a) Comparison of the one, two or three channel RGB images produced in Step 2.i above with the classification map of the *.*gis* image produced by the cluster analysis. This helps correlate the various cluster to mineral species.

b) Using the table output of the text window to numerically correlate cluster classes with mineral species. This is done by using prior knowledge of the approximate relative proportion of minerals to correlate mineral species with the pixel count of a cluster class, and using channel means as an indication of the chemical composition represented by a cluster class. Use of this table is explained below. This table should be copied and pasted to a spreadsheets to facilitate later edge-effect reassignment and summation. Insert the element name above the appropriate channel from the sequential list made in Step 1.i above, as shown in Table 5.

4b.*i. Display the *.gis image*.

Use *File > Open image* to open the *.gis file.

which displays an image of the sample area in which clusters are shown in different colours. A legend to the left of the image relates the colours to the cluster number (Fig. 33)

4b. ii. *Assign the largest cluster areas to a mineral species).*

Inspect the "%" column in the cluster summary table (Table 5) to see what clusters have the largest areas. These are probably the most common minerals in the image area. What mineral these clusters represent can be surmised both from:

a) looking at the channel means values in the spreadsheet. A number >200, and usually >220, signifies that the element represented by the channel is a major constituent of the mineral. From this information the mineral species should be identifiable. For example, the cluster representing quartz will have a high value for Si, but low values for other elements. A cluster representing muscovite will have high values for K and Al compared to other elements.

b) comparing the distribution of the cluster of to the distribution of a mineral deduced from the exercise in Step 2.i above and the images saved into a library. .

When the mineral species has been decided upon, change the colour of the cluster on the *.*gis* image to the colour that is desired for the final diagram by double-clicking the colour square in the legend and selecting from the palette that appears.

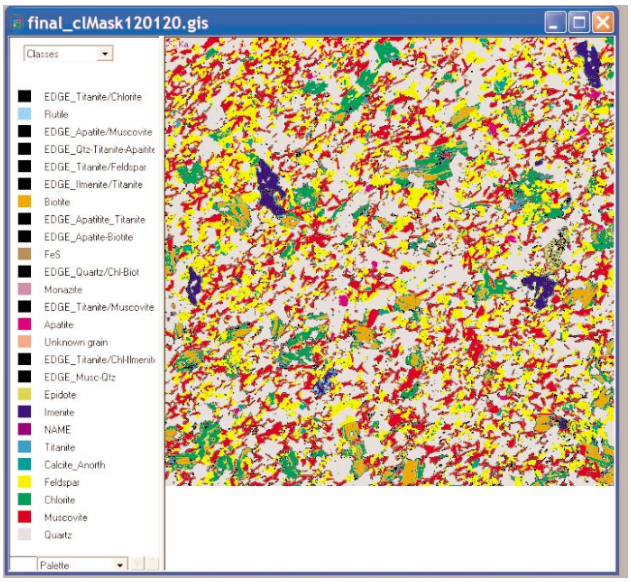


Fig. 33. A **.gis* image produced by a cluster analysis in which all the clusters have been assigned to a mineral class or an edge effect. Note that all edge-effect pixels have been coloured balck.

Change the description of the colour from "Cluster x) to the mineral name by double clicking on the text. Before clicking on "OK" to save the mineral name, copy and paste it into the spreadsheets in a "Class name" column at the appropriate line of the summary statistics in the spreadsheet.

Repeat this for all other clusters that occupy a relatively large area. In some cases, especially where the number of clusters is large, the same mineral may be represented by more than one cluster.

4b. iii. Assign clusters representing minor minerals

Inspect the summary statistics table for the maximum value of minor elements, such as Ti, P, Mn, S. Cluster containing the maximum values are likely minor minerals containing high contents of these minor whole rock elements, such as ilmenite, titanite, apatite, pyrite, etc. The mineral species can likely be identified by inspecting for other high elements in the cluster. For example, ilmenite will have high Fe as well as high Ti, and titanite will have high Ca as well as high Ti. Change colours and text as above.

4b. iv. *Assign clusters representing edge effects.*

If all pixels mapping mineral grains have been assigned to a mineral species, then the remaining pixels are either edge effects, a previously unrecognized mineral class, or minor compositional variants within grains. A procedure for ease of identification of the contexts of these edge effect clusters is to first change the colours of all unassigned clusters on the **.gis* image to white. Then select an unassigned cluster and change its colour to black. The locations of pixels belonging to this cluster are then easily seen on the **.gis* image (zoom in if necessary). Record on the spreadsheet what the cluster represents. For example, a notation EDGE_Qtz/Musc means that the cluster is an edge occurring at the contact between quartz and

MINERAL CLASS.	MINERAL GRAINS.	EDGE Titanite/Muscovite	EDGE Titanite/Feldspar	EDGE Titan/Chl-Ilm	EDGE Qtz/Titanite-Apatite	EDGE Qtz/Chl-Biot	EDGE Musc/Qtz	EDGE Ilmenite/Titanite	EDGE Chlorite/Titanite	EDGE Apatite/Musc	EDGE Apatite/Titanite	EDGE Apatite/Biotite	Total	%
Edge effect pixels	36691	*696*	*390*	*1560*	*1918*	*7889*	*23464*	*23*	*420*	*242*	*26*	*63*		
Unknown	63												63	0.02
Titanite	1293	348	195	780	504			12	210		13		3354	1.28
Rutile	72												72	0.03
Quartz	98903				959	3945	11732						115539	44.07
Muscovite	44261	348					11732			121			56462	21.54
Monazite	86												86	0.03
Ilmenite	2715			123				12					2849	1.09
FeS	108												108	0.04
Feldspar	49385		195										49580	18.91
Epidote	766												766	0.29
Chlorite	14556			657		2494			210				17918	6.84
Calcite	3540												3540	1.35
Biotite	8463					1450						32	9945	3.79
Apatite	1168				455					121	13	32	1789	0.68
NAME2	14												14	0.01
NAME	37												37	0.01
TOTAL	262121												262121	99.99

Table 6. A matrix of pixel counts of mineral classes versus edge effects in a spreadsheet. The edge effect pixels (in italics) are assigned equally between mineral classes of a binary effect but in proportion to the area of the mineral class (second column) for a multi-mineral edge effect (e.g. for the Qtz/Titanite-Apatite edge effect class, 50% of the pixels are assigned to quartz, and the remaining 50% to titanite and apaitite in proportion to the number of pixels in the second column. Note the discrepancy between the total number of pixels (262,121) and the total number of pixels in the image(262.144) is due to the elimination of clusters (by an ISODATA method) with fewer than the minimum cluster size set in Fig.31.

muscovite grains; a notation EDGE_Musc/Qtz-Feld is an edge effect between muscovite and both quartz and feldspar; and a notation INT_Qtz means that the pixels represent some variation within quartz grains. After recording the information in the spreadsheet, change the colour of the cluster back to white and move on to the next cluster, repeating the procedure described above.

The judgement of what a edge effect cluster represents is of course not a precise classification. Although 80% or more of pixels of an edge effect cluster may occur in the context described for them, the remaining pixels may be scattered over the image area and their actual mineralogical context remains uncertain. This is a source of uncertainty in the method.

4b.iv. Calculate areas of mineral species.

Via a matrix on the spreadsheet, such as the one in Table 6, sum the pixels attributed to each mineral species. This summation includes the clusters attributed to mineral grains and a proportional share of those edge effect clusters in which the mineral species is an end member. For binary edge effects (e.g. EDGE_Qtz/Musc) the pixels of the edge effect cluster are evenly distributed between the two end members. For more complex edge effects a proportional distribution is made. For example, for an EDGE_Musc/Qtz-Feld edge effect, 50% of the pixels are assigned to muscovite, and the remaining 50% is assigned to quartz and feldspar in proportion to the pixel count of their respective mineral grain clusters. The accuracy of this method of assigning edge-effect pixels to a mineral species cannot be determined, and is an additional source of uncertainty to the method. A table for the modal mineralogical analysis can be constructed from the first and last columns in Table 6.

3.5. Supervised classification by the training fields method.

An alternative to the cluster analysis method for classifying the pixels into mineral species, is to use small training sets to define the cluster parameters which are then applied to the entire image area. The advantage of this method is that edge-effect pixels are mathematically assigned to the nearest pixel cluster, removing the subjectivity

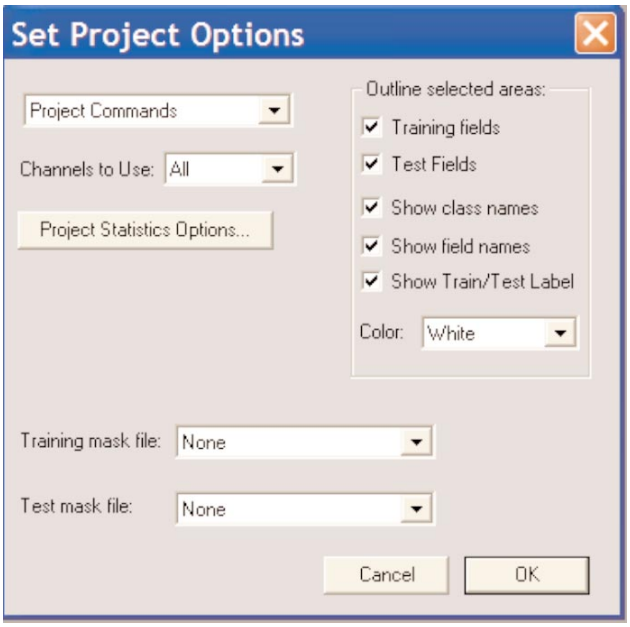


Fig. 34. The “Set Project Options” window which opens with the *Processor->Statistic*s command.

associated with assignment by the user. An imperative of this method is that the user should know where in the image examples of all mineral classes occur.

3. 5.1 Select training fields for each mineral class.

:i) With the *.lan image window active (i.e. selected so that the title bar is dark blue), apply the *Processor->Statistics.* command. A "Set Project Options" window will appear. Set the options as in Fig. 34 i.e.

Channels to use: All

Outline selected areas: check all options. These provide a graphical record on the *.lan image as to where the various training fields are located on the image.

Colour: White is generally easier to read on a multi-coloured background.

Training mask file: None

Test mask file: None

By Clicking “OK” a Project window will appear (Fig. 35). With the *.lan image set to the 1, 2 or 3 channels that best displays the mineral of interest, and with the Project window set as :

Class: "New"

Outline a rectangular area of the selected mineral by dragging the cursor, or by checking the

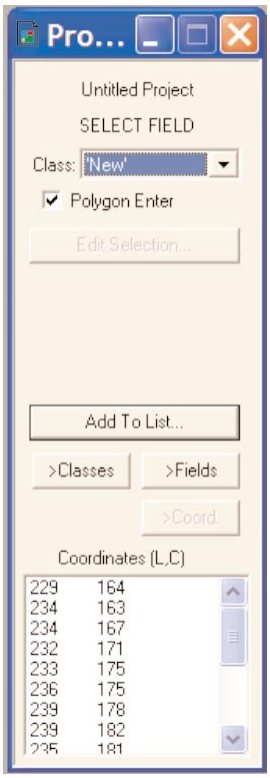


Fig. 35 The "Project" window.

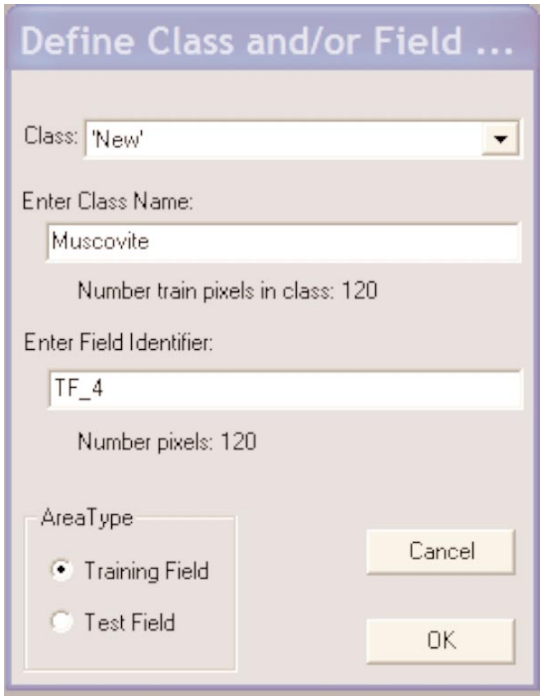


Fig. 36 The "Define Class and/or Field"" window which opens after selecting a training field on the **.lan* image and the "Add to List" button is clicked in the Project window (Fig. 35).

"Polygon enter" option in the Project window, outline an irregular area of the mineral by successive clicking to define the points of a polygon. Click the "Add to list" button in the "Project" window and a "Define Class and/or Field" window will appear.(Fig 36)..

Enter Class Name: Fill in the name of the mineral

Enter field identifier: Fill in as desired such as the default "Field 1" or something more abbreviated such as simply "1"

Note that the number of pixels in this field is listed in the window.

Area type: Check Training field:

By clicking OK the training area and the class and field names are written on the **.lan* image in white.

Repeat selecting 3-4 different fields for the same mineral until >200 pixels have been selected. The minimum total number of pixels is the number of different minerals plus one. After each selection the default Class in the Project window is the current class for which the training areas are being selected.

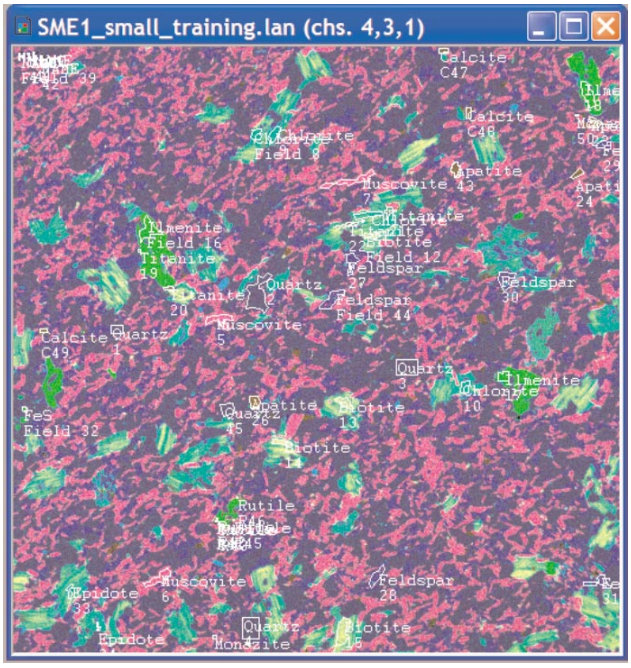


Fig. 37. A **.lan* image after completing selection of training fields.

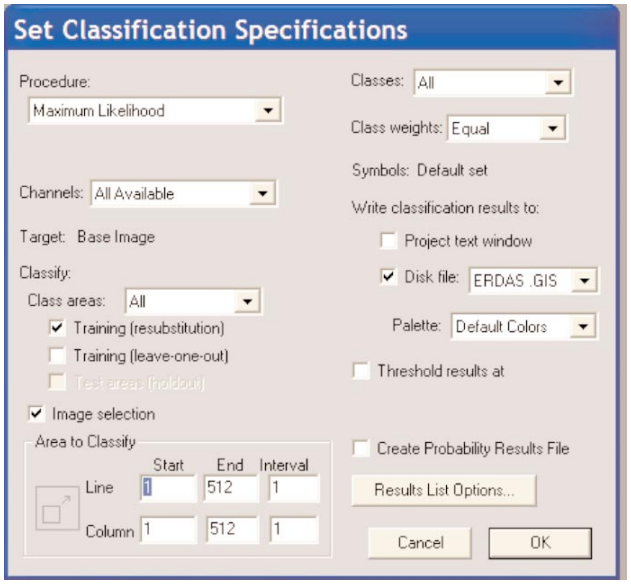


Fig. 38 The "Set Classification Specifications"" window which opens with the Processor->Classify command.

Select training fields for the next mineral by selecting "New" from the drop-down menu of the Class frame of the Project window and repeating the steps above.

After selecting all the training fields, the *lan image will look something like Fig. 37 in which the locations of all training fields are marked in white. These fields can be edited via the "Project" window (Fig. 35) by successively clicking on the appropriate buttons.

3.5.2. Choose the classification method for mapping the mineral classes.

With the *.lan image window active select apply the *Processor -> Classify* command. A "Set Classification Specification Window" will appear (Fig. 38). Select the following options:

Procedure: The Minimum Euclidean Distance, Fisher Linear Discriminant, and the CEM (Constrained Energy Minimization) methods seem to give results that are most consistent with greyscale segmentation methods.

Channels: All available

Class areas: All

Check *Training (resubstitution)*

Check *Image selection*

Area to classify: Line: Start 1 End 512 Interval 1 Column; Start 1 End 512 Interval 1

Classes: All

Class weights: Equal

Write classification results to: Check Disk file and use the ERDAS.GIS format Default Colors for *Palette*.

Do not check *Threshold results at* or *Create Probability* results file.

Results list options: Check all options under Training Areas

Click OK

A *Save Classification as:* window appears. Type in the name that you wish for this **.gis* file. Click Save.

(If the *Create Probability results file* has been selected a "save Probability map as" window will appear. Type in the name that you wish for this **.gis* file. Click Save. This type of image is not used for current purposes).

3.5.3. Classification reliability.

Check the classification accuracy by inspecting the "Training Class Performance" (lists individual training areas) and "Summary Training Class Performance" (conveniently lists classes by mineral name" in the Text window.

In the "Summary Training Class Performance" it is desirable that the Reference Accuracy and the "Reliability Accuracy" both be > 98% for each class.

If this is not the case, look for those training areas which have an undue proportion of reclassified pixels in the "Training Class Performance". Inspect these areas on the **.lan* image to see if the training area could be improved upon (e.g whether the training area crosses grain boundaries; whether it has inclusions; etc). Also check to make sure that every mineral occupying > 5% of the image area has been given a training field.

If necessary, delete the offending training field by:

i) In the Project window, click the "Classes" button and double-clicking the mineral class from the drop down list.

ii) Select the training field from the "Fields" drop down list that will appear.

ii) Select *Edit-> Cut Field* from the main menu bar.

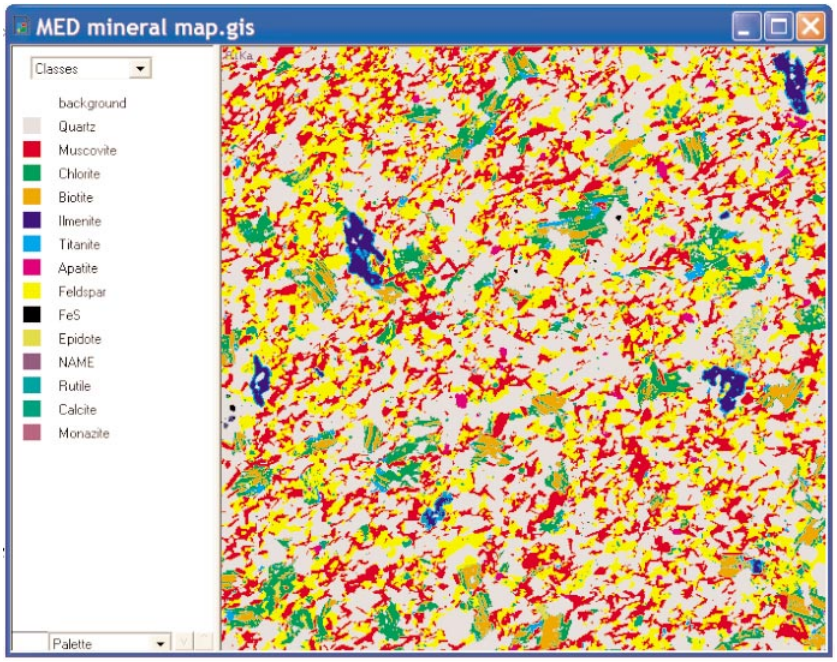


Fig. 39. A mineral distribution map produced from the training fields of Fig. 37 and the Minimum Euclidian Distance classifier. Compared to Fig. 33. which was produced by a cluster analysis, this image has assigned all pixels to a mineral class and the legend is produced in its final form by the software.

iii) Re-define the training area.

iv) When all changes, if any, have been made, click on the "Update Project Stats" button in the Project window.. If you forget to do this "An "Update Project statistics before continuing" window will likely appear when you attempt to reclassify the image.

3.6. Production of a table of results and a mineral distribution map.

Open the **.gis* image. (Fig. 39). This will be a map of the image area with each mineral class coloured as per legend. Change the colour of the mineral class on the **.gis* image to the colour that is desired for the final diagram by double-clicking the colour square in the legend and selecting from the palette that appears. Save the image as a *.tif file for future use, but notice that the legend is not saved with the image area. Details of the legend are saved with the Project file (**.prj*).

Copy the distribution statistics table "CLASS DISTRIBUTION FOR SELECTED AREA" from the text window and paste into a spreadsheet for future use. The area fraction of each mineral in the results table of the Text window is reported to only one place of decimal. To calculate the area fraction to two places of decimal the pixel count should be copied into a spreadsheet and normalized to the total number of pixels in the image area.

Mineral Class	Area %
Apatite	0.52
Biotite	3.08
Calcite	0.80
Chlorite	6.19
Epidote	0.49
Feldspar	21.56
FeS	0.04
Ilmenite	1.10
Monazite	0.04
Muscovite	21.79
Quartz	43.13
Rutile	0.03
Text	0.02
Titanite	1.21
Total	100.00

Table 7. A modal mineralogical analysis of the mineral classes shown in Fig.39 produced by the Training Fields method and Minimum Euclidian Distance classifier using Multispec©.

3.7. Comparison of Multispec methods.

The Training Field method is much faster than using cluster analysis, but requires a thorough knowledge of all the minerals occurring in the image area.

4. CORRECTION OF X-RAY MAPS FOR INSTRUMENT DRIFT.

4. Introduction

The collection of X-Ray counts for a complete X-Ray map may take as much as 12-14 hours, depending upon the dwell time set for the electron beam for each pixel position. During this time, there may be an instrument drift, which results in a change in the relationship between the X-Ray count and the concentration of an element in the sample. The most common cause found for this is deterioration of the tungsten filament of the electron gun, especially towards the end of the filament life, which causes a gradual decrease in beam current.

The dwell positions of the electron beam progress sequentially from the top to the bottom of the image area. Consequently, if instrument drift is severe, there is a progressive change in the greyscale ranges for the same elements of the same mineral from the top to the bottom of the image. This could result in an erroneous classification of the image area by both statistical clustering or image segmentation based on the raw greyscale values.

4.1. Symptoms of instrument drift

1.1. Polarity of peak heights along a greyscale profile

A quick test for whether there is significant systematic instrument drift during collection of the X-Ray data is to draw a profile from the top to the bottom of an X-Ray map for a major element of a mineral that is more or less evenly distributed over the image area. Usually Si or Al is a good choice. This can be done in ImageJ by selecting the line tool to draw a vertical line across the image, and using the *Analyse->Plot Profile* command. (Note: a better-labeled version of the ImageJ profile, as in Fig. 40, can be produced by clicking the List button of the profile window; then the Edit button of the Plot Values window; then selecting Copy All and pasting the data into a graphics application). A profile that indicates no significant instrument drift (Fig. 40a) is characterized by the same range of greyscale values for the same peaks and plateaux ranges (see p. 7) from the top (low pixel

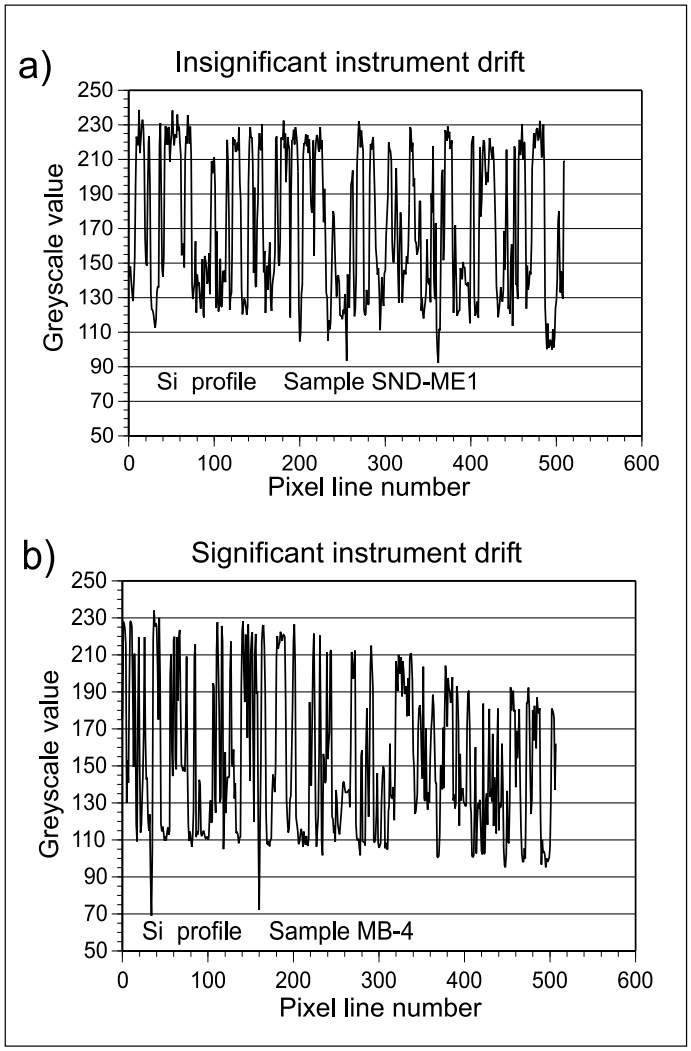


Fig. 40. Profiles of greyscale values along a vertical line across X-Ray maps for Si of fine-grained quartzitic rocks.
a) A case where there is no significant instrument drift. Peaks and plateaux have the same range of greyscale values along the entire length of the profile.;
b) a case where there is significant instrument drift. There is a gradual decrease in peak and plateau values beginning at about Pixel line number 200 to the bottom of the image at Pixel line number 512.

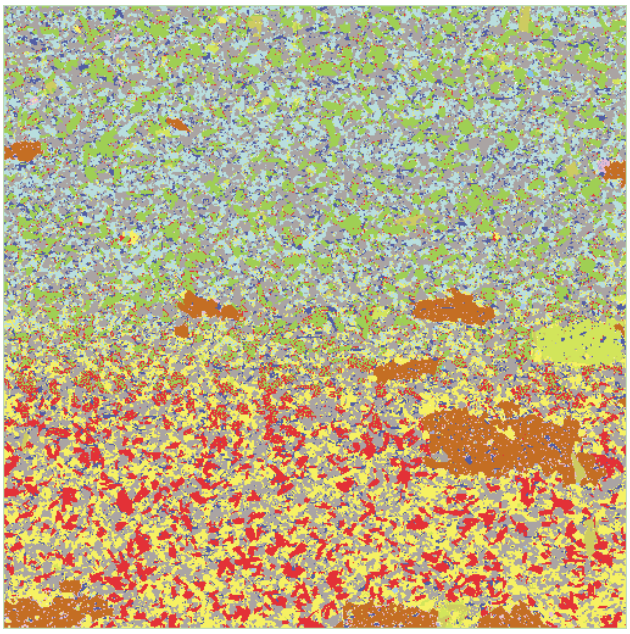


Fig. 41. A mineralogical map of a fine-grained quartzitic sediment (sample MB-4) obtained by using the single pass cluster analysis routine of Multispec© using 10 channels of the same drift-affected X-Ray maps illustrated in Fig. 40 and Fig. 42. Each colour represents a significantly different statistical compositional class. The horizontal "mineralogical layering" is an artifact of instrument drift.

line numbers) to the bottom (high pixel line numbers) of the image. In contrast, a profile that indicates significant systematic instrument drift (Fig. 40b) shows a progressive migration of peak and plateaux greyscale values as a function of pixel line number.

1.2. Horizontal compositional layering on a mineral classification image.

A mineralogical classification map based on a series of X-Ray maps affected by significant instrument drift may show horizontal "mineralogical layering". Fig. 41 is an extreme example. The mean greyscale values for Si, Al and K in muscovite are 113.5, 134.7 and 175.8 respectively in the upper part of the image but 109.5, 122.5 and 152.7 in the lower part of the image. These differences result in muscovite being classified by a cluster analysis as two statistically different minerals. These "minerals" are coloured green (in the upper part of the image) and red (in the lower part of the image) respectively. Similarly feldspar is coloured light blue in the upper part of the image but yellow in the lower part. On the other hand, quartz (which is the only mineral with a high Si X-Ray count but low X-Ray counts for all other elements) and pyrrhotite (the only mineral with a

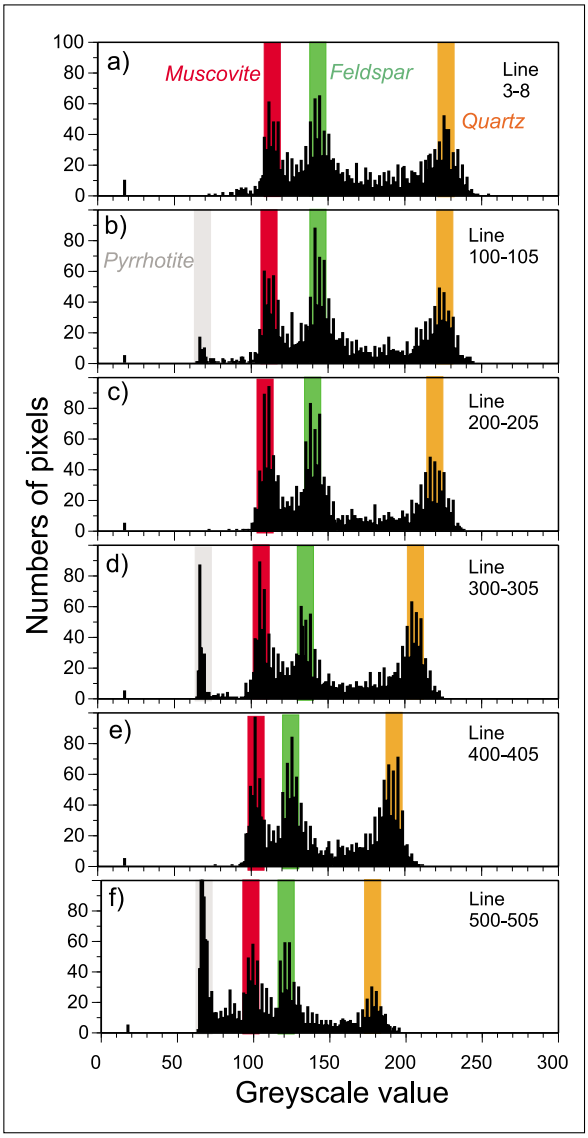


Fig. 42. Histograms of the greyscale values of pixels of the Si X-Ray map for the image shown in Fig. 41. The histograms are for 5 pixel wide horizontal strips across the image, that are spaced at about 100 pixels (pixel line numbers increase from the top to the bottom of the image). The coloured columns show the plateau greyscale range for common minerals in the sample. Note that the plateau range systematically migrates to lower values towards the bottom of the image beginning below pixel lines 100-105.

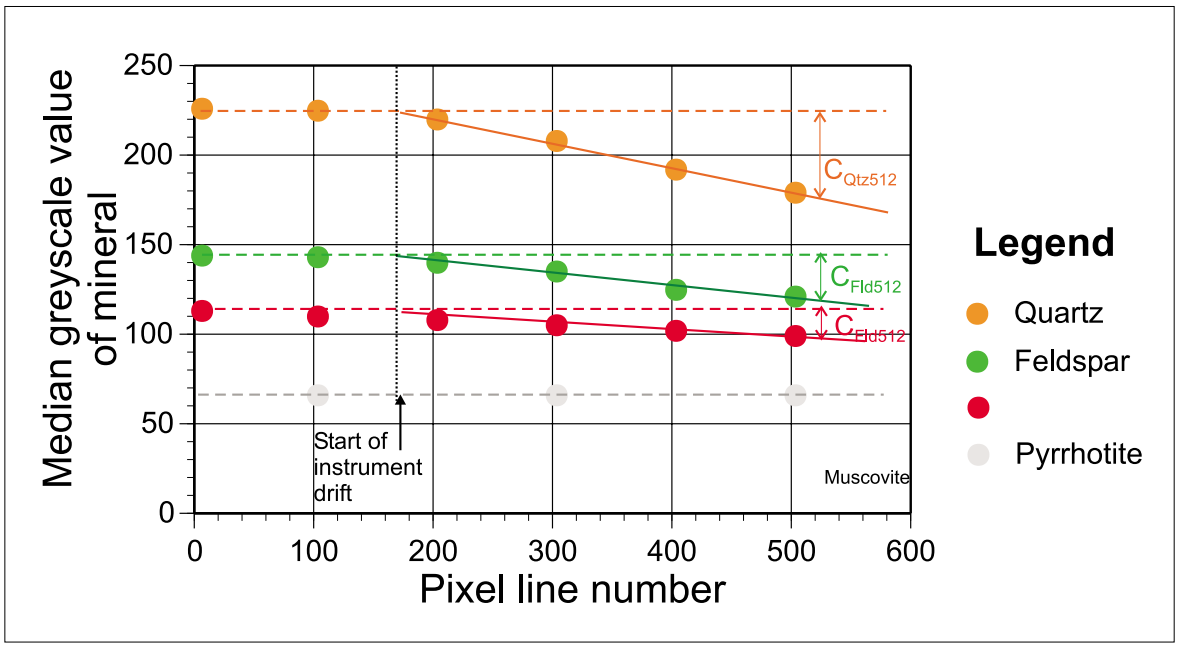


Fig. 43. Plot of average greyscale value (coloured filled circles) of the plateaux ranges shown by the coloured columns in Fig. 42 versus pixel line number. The dashed horizontal is the median greyscale value of the plateau range of the mineral if there were no instrument drift. Samples which have been affected by instrument drift plot below this line and show a sensibly linear correlation (solid colour line) with pixel line number (i.e. with time). The correction needed to compensate greyscale values for instrument drift is the difference between the dashed line and the solid line a The amounts of correction are illustrated for pixel line 512 by the double arrows, which graphically illustrate that the amount of correction is dependent on the greyscale value.

high S X-Ray count) are coloured grey and brown respectively across the image.

4.2. Quantification of instrument drift.

2.1. Migration of greyscale values as a function of pixel line number.

The amount of migration of greyscale values as due to instrument drift is more quantitatively assessed by plotting histograms of horizontal segments of the image spaced at intervals over the vertical height of the image, as illustrated for Si in Fig. 42. These histograms can be produced in ImageJ by using the rectangular select tool to select the desired contiguous pixel line numbers, and then the Analyse->Histogram command. As with the vertical profile described above, a better-labeled version of the ImageJ profile can be produced by clicking the List button of the histogram window; then the Edit ->Copy All of the histogram data window, and pasting the data into a graphics application. The coloured bars of Fig. 42 show the Si plateaux ranges (i.e. the range of the most common greyscale values for the specified mineral on the Si X-Ray map) for the main minerals in the sample. The plateaux ranges for all minerals containing Si systematically decrease with increasing pixel line number (i.e. from the top to the bottom of the image), starting between pixel line 105 and pixel line 200. However, for areas of the image where Si is zero (e.g.. areas occupied by pyrrhotite) pixel greyscale values do not migrate, illustrating that the background count is not significantly affected by instrument drift.

The amount of migration of the plateau range greyscale values of Si for each mineral is sensibly a linear function of the pixel line number (Fig. 43), starting with the pixel line number at which instrument drift begins to have significant impact (about line 185 in Fig. 43).

4.2.2. Migration of greyscale values as a function of raw greyscale value.

To achieve a uniform range of plateau range for each mineral across the entire image area, the measured greyscale values (shown by filled

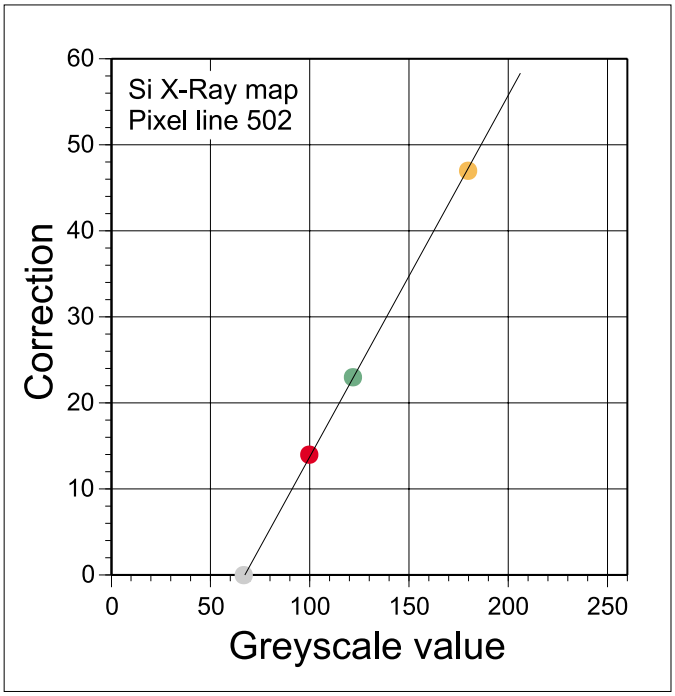


Fig. 44. Plot of correction versus measured greyscale value for Si at line 502 of the image shown in Figs 41-43, showing the sensibly linear relationship between the two. The correction is the difference between the measured greyscale value of an average plateau range of a mineral (represented by the solid coloured lines in Fig. 42) and the greyscale value that the mineral should have displayed at that pixel line number in the absence of instrument drift (represented by the dashed coloured lines in Fig. 43).

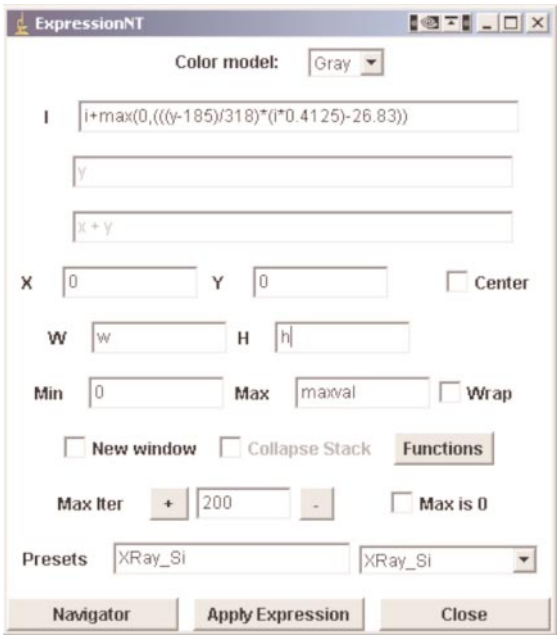


Fig. 45. The ExpressionNT window. Selecting the "Gray" Color Model in the top drop-down window activates only the top of the three windows, which defines the value of "i", the greyscale value f the current pixel. The expression in this window can be entered from the keyboard, and optionally saved as a "Preset", from which it can be later retrieved by use of the Presets dropdown at the bottom of the window. All other parameters should be set as shown, which applies the formula to all pixels in the last-selected *.tif X-Ray map, or to an area of that X-Ray map that has been selected with the rectangular select tool.

coloured circles in Fig. 43) must be corrected by the amount of migration.

The amount of correction to the greyscale value of a pixel is the difference between the measured greyscale value of a plateau range within the area affected by instrument drift (represented by the solid coloured lines in Fig. 43) and the greyscale value that the plateau range would have had if there were no instrument drift (represented by the coloured dashed lines in Fig. 43). The amounts of correction required at pixel line 512, for example, is graphically shown by the double-headed arrowed lines in Fig. 43. As illustrated by Fig. 44 for pixel line 502, the correction at any given pixel line number is sensibly a linear function of the measured greyscale value.

4.3. Compensation for instrument drift for a single X-Ray map.

The effect of instrument drift can therefore be sensibly compensated for by using the two linear relationships discussed above to adjust the greyscale values of the original X-Ray map. A plugin for ImageJ (ExpressionNT) allows the user to define an expression which defines/modifies the value of every greyscale pixel of the image area (see Fig. 45). A suitable expression for this plugin is:

$$i+\max(0,(((y-L_S)/(L_D-L_S)*(i*SLOPE)+INTERCEPT)) \quad 1)$$

where:

i = current greyscale value of pixel

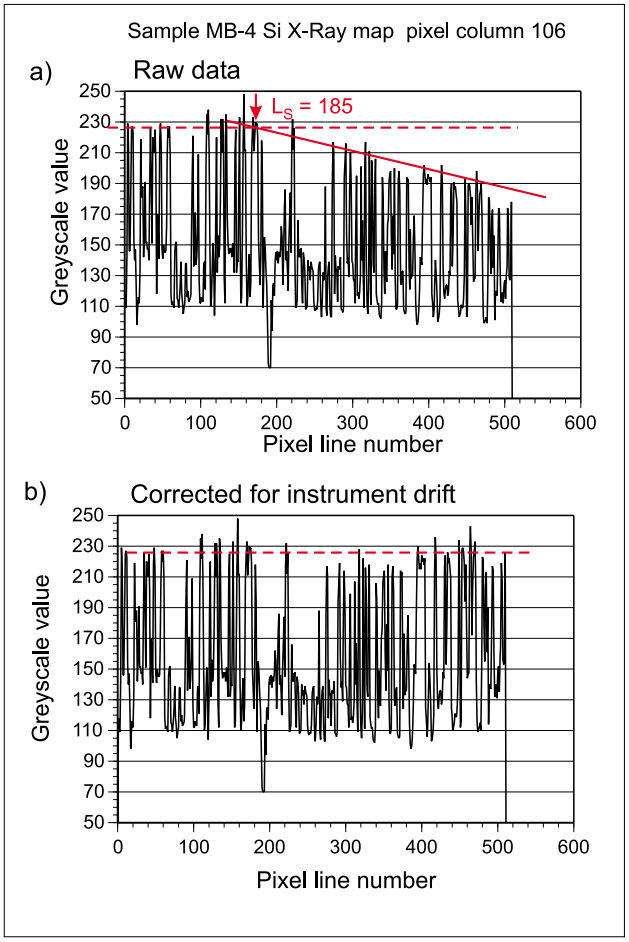


Fig. 46. a) Profile of greyscale values along a vertical line (pixel column 106) of an X-Ray map for Si that shows instrument drift, as in Fig. 40b. The dashed horizontal red line is through the average peak height for quartz for that part of the profile in which there is no instrument drift in the early part of the X-Ray count collection process (low pixel line numbers on the left of the profile). The solid red line is through the average peak height for quartz for that part of the profile in which there is significant instrument drift in the later part of the X-Ray count collection process (high pixel line numbers on the right of the profile). The intersection of the two lines indicates the pixel line number at which significant instrument drift begins and is parameter LS in equation 1 of the text.
b) The same profile as in a) that has been corrected for instrument drift by using equation 2 in the text with the ExpressionNT plugin. Note that the instrument drift effect has been removed and that the average peak height for quartz (dashed red line) now has the same value across the profile.

y = current line number of image

L_S = line number of image at which instrument drift starts

L_D = line number of image used to construct a plot analogous to Fig. 44 (i.e. a plot showing the greyscale value of two or more mineral plateaux at specified line in the image versus the correction that must be added to these values to compensate for instrument drift).

SLOPE = Slope of straight line fit to data of diagram analogous to Fig. 44

INTERCEPT = Intercept on the y axis of straight line fit to data of diagram analogous to Fig. 44

The expression in Equation 1 is not the syntax required by the Expression NT plugin. The terms L_S, (L_D-L_S), SLOPE and INTERCEPT must be numerically evaluated prior to entering the expression (see below). For the example of Si illustrated in Fig. 40 through 44, the syntax required by Expression NT is:

i+max(0,(((y-185)/318)*(i*0.4125)-26.83)) *2)*

It is not necessary to produce all the diagrams shown here (Figs. 40-44) to obtain the data required to compensate an X-Ray map for instrument drift. Only two diagrams are necessary:

i. A vertical profile of greyscale values (Fig. 46), which is required to determine whether there is any significant instrument drift in the first place (see Fig. 40). The parameter L_D can be determined by drawing a horizontal line through peak heights at low pixel line numbers (horizontal red dashed line in Fig. 46) and a solid line through analogous peak heights (sloped red solid line in Fig. 46) at high pixel line numbers. The two lines intersect where significant instrument drift begins, and the pixel line number for the beginning of instrument drift (parameter L_D) can be read off the horizontal axis of the diagram.

ii. Two histograms of greyscale values of a single pixel line, or over a small range of line numbers, such as in Fig. 47. One of the histograms must be of a pixel line within the area of the image not significantly affected by instrument drift i.e. the pixel line number < L_D (Fig. 47a), from which the median plateau greyscale value for two minerals

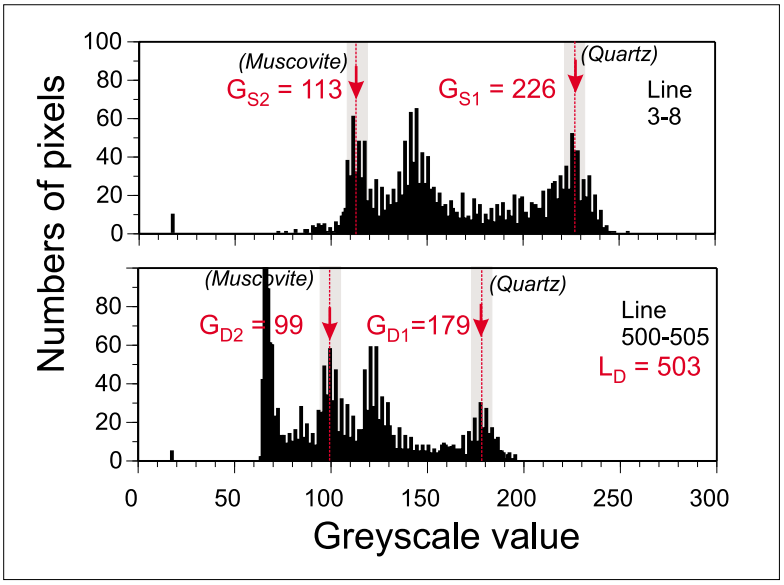


Fig. 47. Histograms of the greyscale values of pixels of the Si X-Ray map for pixel lines 3-8 (in stable part of X-Ray map) and pixel lines 500-505 (in part of X-Ray map affected by instrument drift) reproduced from Fig. 42, showing the measurement of parameters G_{S1}, G_{S2}, G_{D1}, G_{D2}, L_D required for equations 3 and 4 of text.

are determined (G_{S1} and G_{S2} respectively, the suffix "S" denoting the stable part of the image). The other histogram must be of a pixel line within the area of the image that has been affected by instrument drift i.e. the pixel line number > L_D (Fig. 47b), from which the median plateau greyscale value for the same two minerals are determined (G_{D1} and G_{D2} respectively, the suffix "D" denoting the part of the image affected bi instrument drift).

The SLOPE parameter in equation 1) above is given by:

$$SLOPE = ((G_{S1}-G_{D1})-(G_{S2}-G_{D2}))/(G_{D1}-G_{D2}) \quad 3)$$

and the INTERCEPT parameter in equation 1) above is given by:

$$INTERCEPT = 0-((((G_{S1}-G_{D1})*G_{D2})-(G_{D1}*(G_{S2}-G_{D2})))/(G_{D1}-G_{D2})) \quad 4)$$

Equations 3 and 4 can be evaluated separately in a spreadsheet, and the numerical values for SLOPE and INTERCEPT transcribed into equation 2 for entering into the ExpressionNT plugin.

4.4 Compensation for instrument drift for other X-Ray maps of the same run.

The example discussed above produces values for the L_D, SLOPE and INTERCEPT parameters of equation 1 that are valid only for the Si X-Ray map. The value for parameter LS is the same for all X-Ray maps produced during the same run. The same exercise described in Section 3 above must therefore be repeated for each element X-Ray map to determine values of the LD, SLOPE and INTERCEPT parameters. Values of these parameters for a variety of elements are listed in columns 1 through 9 in Table 2.

4.5. Time-saving approximations.

1. Direct reading of values of L_S, G_{S1}, G_{S2}, G_{D1} and G_{D2} from ImageJ plots.

Estimation of numerical values from graphical plots involves a certain amount of subjectivity. Replotting of ImageJ graphics by a graphics application can help reduce the subjectivity, both by allowing graphical construction lines, as in Fig. 45a, and by the better labeling of the axes of the plots to allow more accurate estimation of values. However, unless high quality graphics are required for other purposes, the value of L_S and the parameters required for equation 3 and equation 4 above

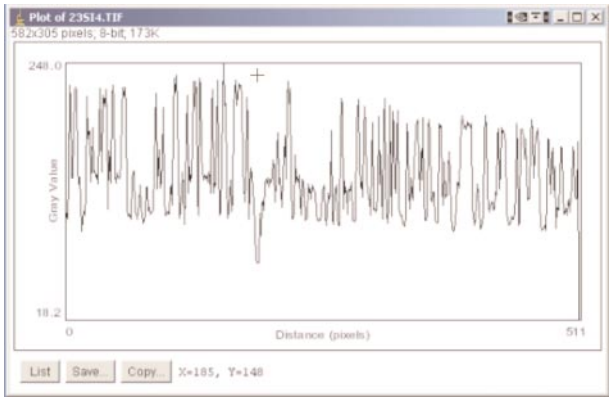


Fig. 48. The *ImageJ* Plot window that appears on using the *Analyze->Plot* Profile command after using the Line select tool to draw a vertical line from the top to the bottom of an X-Ray map for Si. The cursor position, shown by a cross, is marking the inflection point of an imaginary curve through the average peak heights. The pixel line number of the cursor is shown by the X value at the bottom of the window. Note that the Y value is the value on the profile for this pixel line number (pixel distance).

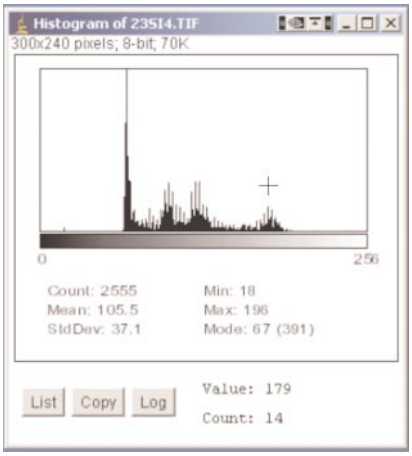


Fig. 49. The *ImageJ* Plot window that appears on using the *Analyze->Histogram* command after using the rectangular select tool to select a number of contiguous pixel lines across the width of an X-Ray map for Si. The cursor position, shown by a cross, is marking the median value of a plateau range for quartz. The greyscale value of this cursor position is given by the Value parameter at the bottom f the window.

can be read directly from the ImageJ versions of Fig. 46a and Fig. 47 respectively. To obtain the value of L_S, move the cursor over the ImageJ profile (when the cursor will change from an arrowhead to a cross), place the cursor cross at the imagined inflection of the line through average peak

1 Element	2 G_{S1}	3 G_{D1}	4 G_{S2}	5 G_{D2}	6 L_S	7 LD	8 Slope	9 Intercept	10 Original greyscale value	11 Pixel row number	12 Corrected greyscale value
Si	226	179	113	99	185	503	0.4125	26.8375	180	512	230
Al	173	146	78	78	185	403	0.3970	30.9705	180	512	225
K	181	154	117	106	185	503	0.3333	24.3333	180	512	232
Ca	248	200	83	78	185	500	0.3524	22.4918	180	512	234
Fe	221	180	86	82	185	503	0.3775	26.9591	180	512	229
Na	94	85	69	67	185	483	0.3888	24.0555	180	512	232
Mg	177	147	78	76	185	483	0.3943	27.9718	180	512	231

Table 8. Values for G_{S1}, G_{S2}, G_{D1}, G_{D2}, L_S and L_D for major elements of the image shown in Fig. 41, and the calculate SLOPE and INTERCEPT parameters from equations 3 and 4 respectively. Column 12 shows the value of the corrected grey scale value of a pixel in row 512 (column 11) with a raw greyscale value of 180 (column 10). Note that most (6 out of 7) corrected greyscale values are in the range 231±3, so that a time-saving approximation is to use the same equation 2 for all elements to correct the effects of systematic instrument drift.

heights, and read the pixel line number from the value of the cursor along the X-axis given at the bottom of the window (Fig. 48). To obtain the values of G_{S1}, G_{S2}, G_{D1} and G_{D2}, move the cursor over the ImageJ histogram of greyscale values for a selected pixel line interval to a position above the median plateau range value for a selected mineral (Fig. 49). The greyscale value of the pixel position is given by the Value parameter at the bottom of the window.

2. Using the same values of L_D, SLOPE and INTERCEPT for all elements.

Column 12 of Table 8 lists the corrected greyscale value of a pixel occurring on pixel line 512 (column 11) with a raw greyscale value of 180 (column 10), using the different values of LD, SLOPE and INTERCEPT listed in columns 7 through 9. The corrected greyscale values range between 225 and 234, which is a small range compared to the shift in greyscale value from 180. Therefore, the use of any one of the sets of values of Table 2 with the Expression NT plugin would greatly improve the quality of the raw X-Ray map. For most cases, it would seem that this improvement is to the point that any further refinement would not have a substantial effect on the final modal mineralogical analysis. A time-saving approximation would therefore be the determination of LS, LD, SLOPE and INTERCEPT for just one X-Ray map and applying the same expression (e.g. equation 2) to all X-Ray maps of the same run.

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ACQUISITION OF SOFTWARE.

MultiSpec©

"MultiSpec© is being developed at Purdue University, West Lafayette, IN, by David Landgrebe and Larry Biehl from the School of Electrical and Computer Engineering, Agronomy and LARS. It results from an on-going multi-year research effort which is intended to define robust and fundamentally based technology for analyzing multispectral and hyperspectral image data, and to transfer this technology to the user community in as rapid a manner as possible. The results of the research are implemented into MultiSpec and made available to the user community via the download pages. MultiSpec© with its documentation© is distributed without charge." (statement from Multispec web page).

The software can be downloaded free of charge from the following web site:

http://dynamo.ecn.purdue.edu/~biehl/MultiSpec/

The software is downloaded as a self-extracting archive, and includes explanatory files. The software is available both as Windows and MacIntosh versions. Additional documentation is available from the web site given above on how to use Multispec and how to interpret multispectral data. "An Introduction to Multispec" by David Landgrebe and Larry Biehl is highly recommended to give the user further explanations and descriptions of Multispec's capabilities than is given in this Open File.

For the convenience of the user of this Open File, copies of the self-extracting archive of the Windows version of Multispec software, and the PDF file ""An Introduction to Multispec" by David Landgrebe and Larry Biehl, that were downloaded during April 2005, are included on this Open File CD.

ImageJ

"ImageJ is a public domain Java image processing program inspired by NIH Image for the Macintosh. It runs, either as an online applet or as a downloadable application, on any computer with a Java 1.1 or later virtual machine. Downloadable distributions are available for Windows, Mac OS, Mac OS X and Linux."

"ImageJ was designed with an open architecture that provides extensibility via Java plugins. Custom acquisition, analysis and processing plug-ins can be developed using ImageJ's built in editor and Java compiler. User-written plugins make it possible to solve almost any image processing or analysis problem."

"ImageJ is being developed on Mac OS X using its built in editor and Java compiler, plus the BBEdit editor and the Ant build tool. The source code is freely available. The author, Wayne Rasband (wayne@codon.nih.gov), is at the Research Services Branch, National Institute of Mental Health, Bethesda, Maryland, USA." - (statements from ImageJ web page."

The ImageJ software and plugins can be downloaded free of charge from the following web site.

http://rsb.info.nih.gov/ij/

The ImageJ v.1.33 download includes Sun's JRE 1.3.1_03 Java runtime environment. A version bundled with Java 1.5 (5.0) is also available. Online documentation for ImageJ software is also available from this web site.

For the convenience of the user of this Open File, a copy of ImageJ v.1.33, and the ExpressionNT plugin by Ulf Dittmer, that were downloaded during April 2005, are included on this Open File CD.

GEOLOGICAL SURVEY OF CANADA

OPEN FILE 4941

The measurement of the modal mineralogy of rocks from SEM imagery: the use of Multispec © and ImageJ freeware

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J.W. Lydon.